

FIG. 1

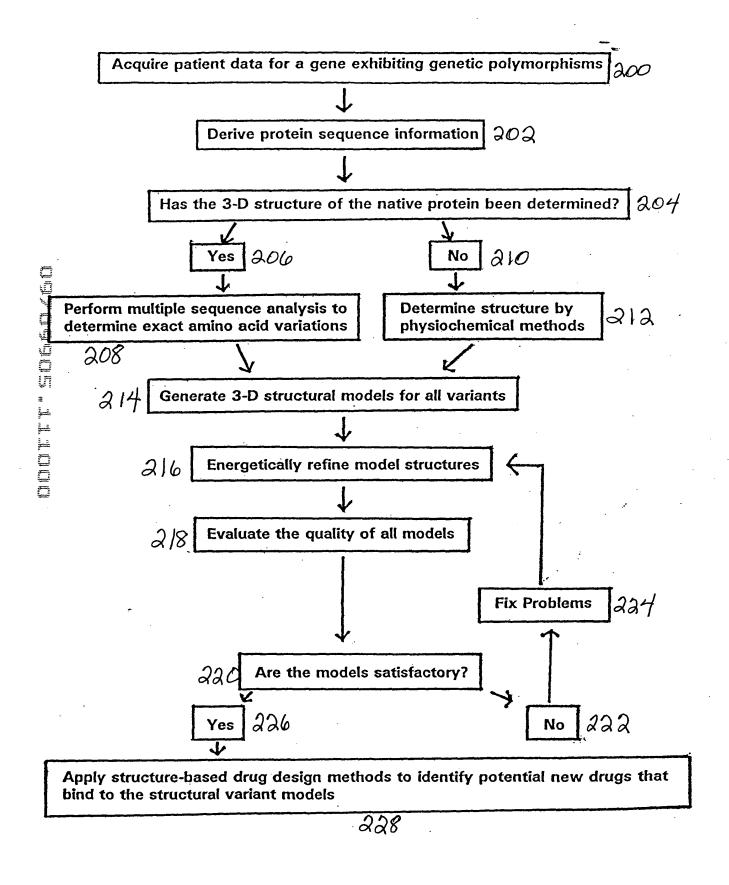
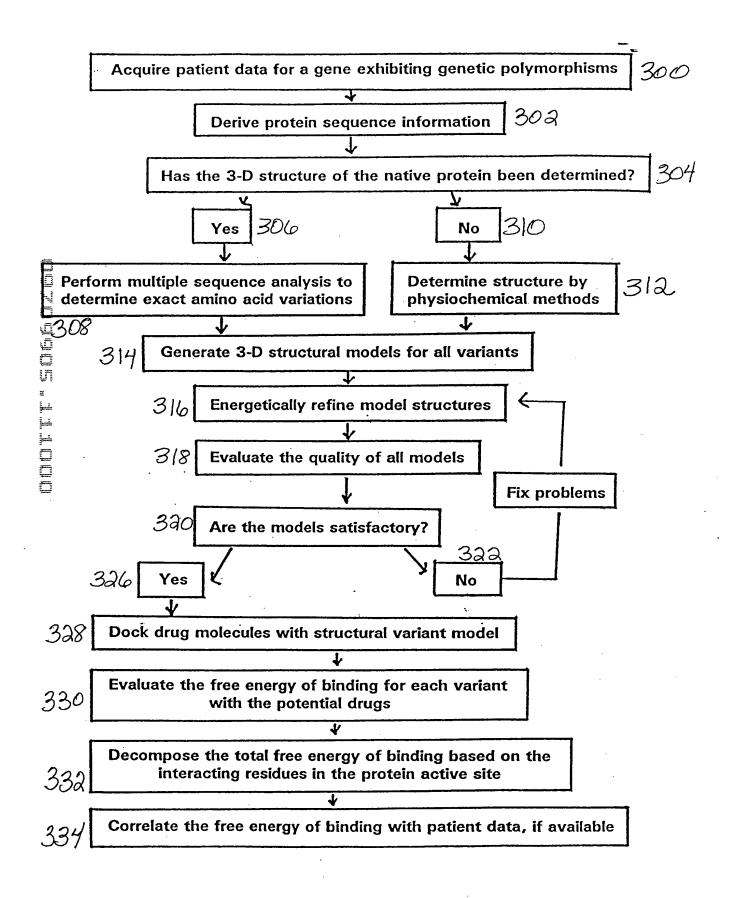


FIG. 2

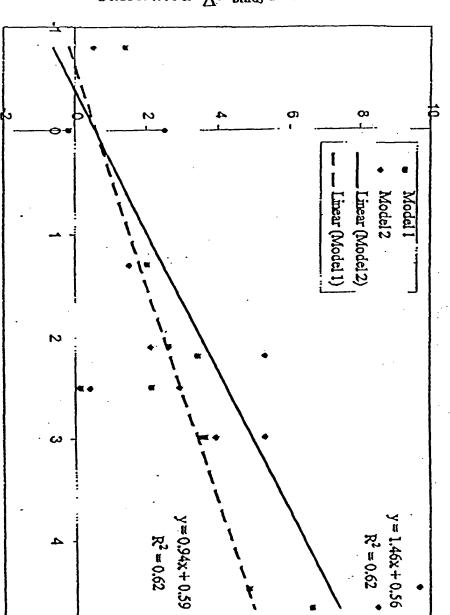


of Binding Energy upon Ligand Modifications in the Binding

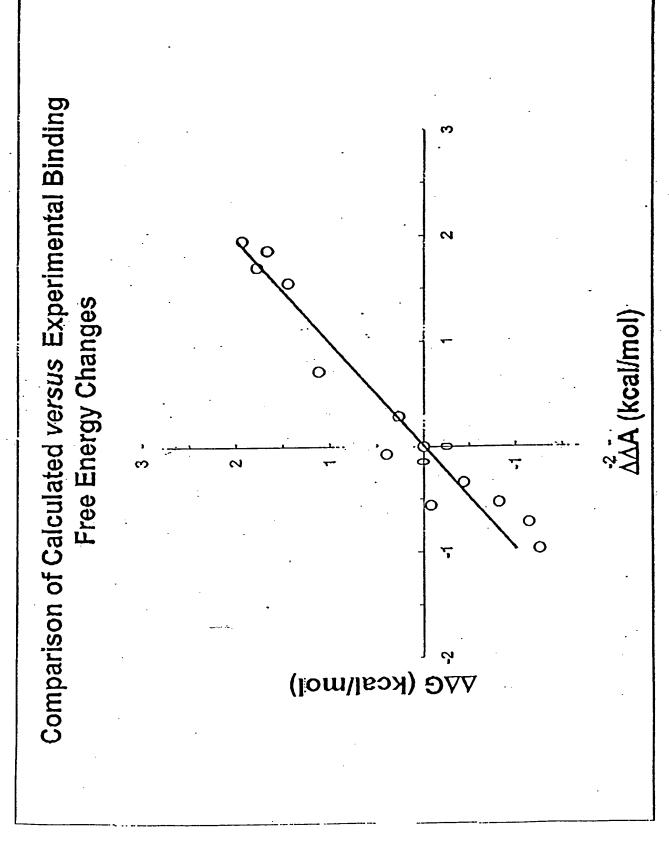
Site of NS3

Correlation between Experimental and Calculated Changes

# Calculated A: Ebiad, kcal/mol



Expected  $\Delta E_{bluo}$  kcal/mol



户16.5

# HIV Protease Inhibitors Approved by FDA

Saquinavir

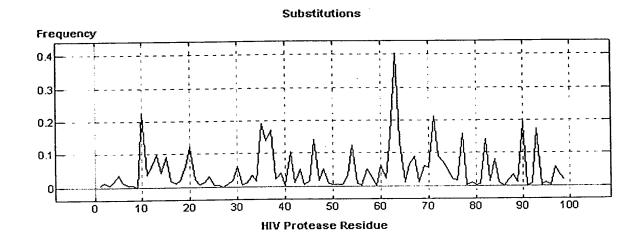
Nelfinavir

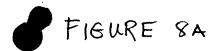
Indinavir

Amprenavir

Ritonavir

# FIGURE 7







Database filename: hivpr.mdb

Number of structures: 10591

Tolerance (%): >= 1,05

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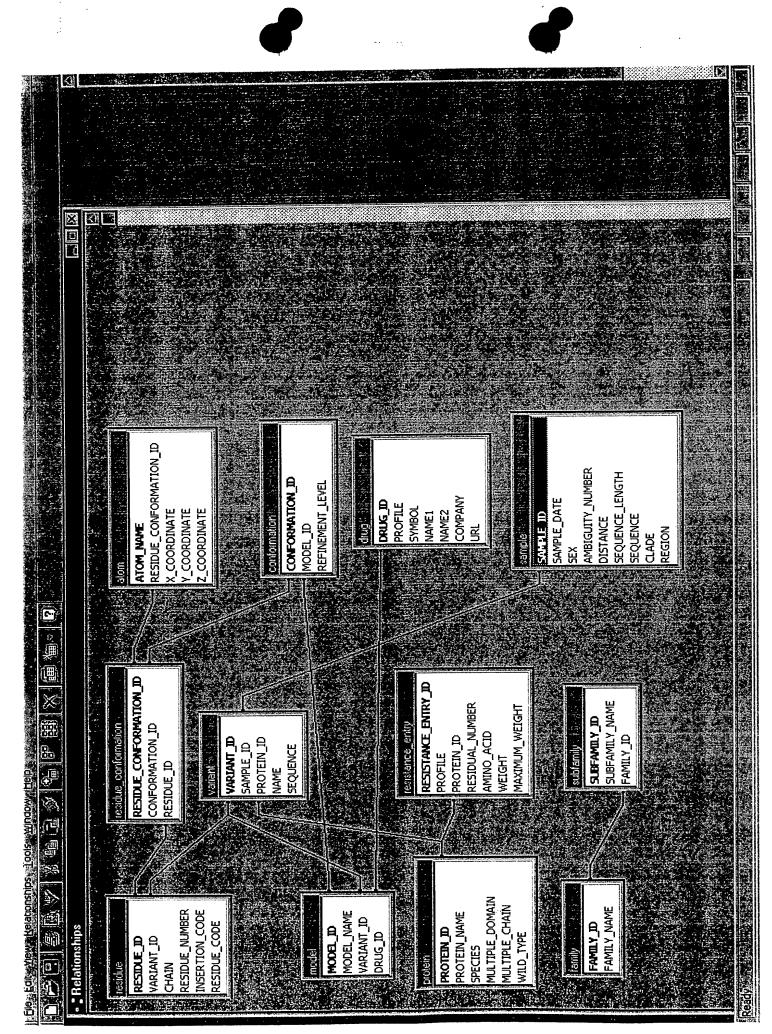
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83	84	85	98	87	88	89	90	91	95	63	94	92	96	26	86	66

FIG. 9







# Figure 11A

MOTA	1	N	PRO	Α	1	-3.433	7.956	34.152
ATOM	2	CA	PRO	Α	1	-2.653	6.918	34.784
ATOM	3	С	PRO	Α	1	-1.242	7.005	34.259
ATOM	4	Ō	PRO	A	1	-0.950	7.638	33.216
ATOM	5	CB	PRO	A	1	-3.281	5.601	34.262
ATOM	6	CG	PRO	A	1	-4.191	5.995	33.118
ATOM	7	CD	PRO	A	1	-4.547	7.461	33.339
ATOM	8	1H	PRO	A	1	-2.845	8.493	33.547
	9	2H			1		8.552	34.853
ATOM				A		-3.824		35.001
ATOM	10	N		A	2	-0.259	6.464	
ATOM	11	H	GLN		2	-0.475	6.057	35.889
ATOM	12	CA	GLN		2	1.115	6.443	34.568
ATOM	13	C	GLN		2	1.452	4.993	34.301
ATOM	14	0	GLN		2	1.379	4.106	35.173
ATOM	15	СВ	$\operatorname{GLN}$		2	2.070	6.966	35.653
MOTA	16	CG	GLN		2	3.549	6.859	35.240
MOTA	17	$^{\rm CD}$		Α	2	4.490	7.744	36.054
MOTA	18	OE1		Α	2	4.771	8.888	35.719
MOTA	19	NE2		Α	2	4.980	7.190	37.144
MOTA	20	1HE2	GLN	Α	2	5.605	7.702	37.734
MOTA	21	2HE2	GLN	Α	2	4.731	6.253	37.390
MOTA	22	N	ILE	Α	3	1.784	4.644	33.037
MOTA	23	H	ILE	Α	3	1.876	5.351	32.336
MOTA	24	CA	ILE	Α	3	2.013	3.257	32.665
ATOM	25	С	ILE	Α	3	3.505	3.028	32.473
ATOM	26	0	ILE	Α	3	4.242	3.777	31.787
ATOM	27	CB		A	3	1.226	2.944	31.370
ATOM	28	CG1	$_{ m ILE}$	Α	3	-0.274	3.239	31.603
ATOM	29	CG2	ILE	A	3	1.427	1.480	30.901
ATOM	30	CD1		A	3	-1.089	3.219	30.322
ATOM	31	N		A	4	4.071	2.032	33.177
ATOM	32	H	THR		4	3.525	1.525	33.844
ATOM	33	CA	THR		4	5.451	1.661	33.007
ATOM	34	C		A	4	5.515	0.637	31.901
ATOM	35	0	THR	A	4	4.490	0.037	31.397
ATOM	36	CB		A		6.051	1.125	34.324
ATOM	37		THR	A	4			
		OG1			4	5.224	0.069	34.791
ATOM	38	HG1		A	4	5.589	-0.299	35.646
ATOM	39	CG2	THR		4	6.085	2.212	35.431
ATOM	40	N	LEU		5	6.677	0.281	31.405
ATOM	41	H	LEU		5	7.518	0.530	31.885
ATOM	42	CA	LEU		5	6.754	-0.464	30.177
ATOM	43	C	LEU		5	7.432	-1.813	30.356
ATOM	44	0	LEU		5	7.940	-2.464	29.426
ATOM	45	CB	LEU		5	7.459	0.394	29.128
ATOM	46	CG	LEU		5	6.668	1.671	28.775
ATOM	47	CD1		Α	5	7.493	2.649	27.939
MOTA	48	CD2		Α	5	5.345	1.307	28.099
ATOM	49	N		A	6	7.420	-2.351	31.594
ATOM	50	H	TRP	Α	6	7.030	-1.833	32.356
ATOM	51	CA	TRP	Α	6	7.958	-3.669	31.865
ATOM	52	C	TRP	Α	6	7.071	-4.697	31.204
ATOM	53	0	TRP	Α	6	7.520	-5.798	30.828
ATOM	54	CB	TRP	Α	6	8.099	-3.913	33.367
ATOM	55	CG		Α	6	9.041	-2.974	34.070





# Figure 11<sub>B</sub>

ATOM	56	CD1	TRP A	A	6	8.745 -1.769 34.646
ATOM	57	CD2	TRP A	A	6	10.449 -3.171 34.273
ATOM	58	NE1	TRP A	A	6	9.875 -1.209 35.190
ATOM	59	HE1	TRP A	A	6	9.930 -0.332 35.668
ATOM	60	CE2		A	6	10.932 -2.048 34.974
ATOM	61	CE3		A	6	11.334 -4.190 33.924
	62	CZ2		A	6	12.257 -1.917 35.333
ATOM		CZ3		A.	6	12.650 -4.065 34.278
ATOM	63					13.106 -2.942 34.974
ATOM	64	CH2		A ~	6	
ATOM	65	N		A	7	
MOTA	66	H		A	7	5.354 -3.619 31.343
ATOM	67	CA		A	7	4.952 -5.339 30.205
MOTA	68	С		A	7	4.438 -4.569 29.033
ATOM	69	0		A	7	4.433 -3.321 29.000
ATOM	70	CB	GLN A	A	7	3.712 -5.693 30.969
ATOM	71	CG	GLN Z	Α	7	4.015 -6.467 32.210
MOTA	72	CD	GLN Z	Α	7	2.734 -6.678 32.917
ATOM	73	OE1	GLN A	Α	7	2.053 -7.681 32.712
ATOM	74	NE2		Α	7	2.356 -5.682 33.736
ATOM	75	1HE2		A	7	1.501 -5.748 34.251
ATOM	76	2HE2		A	7	2.926 -4.867 33.837
ATOM	77	N	ARG A		8	3.777 -5.239 28.078
ATOM	78	H		A	8	3.688 -6.233 28.142
	79	CA		A	8	3.183 -4.568 26.948
ATOM		C	ARG A		8	2.117 -3.648 27.461
ATOM	80					1.333 -3.965 28.387
ATOM	81	O	ARG A		8	
MOTA	82	CB	ARG A		8	2.574 -5.555 25.975
MOTA	83	CG	ARG .		8	3.532 -6.593 25.437
MOTA	84	CD		A	8	2.842 -7.610 24.579
MOTA	85	NE		A	8	3.787 -8.487 23.900
ATOM	86	HE		Α	8	4.762 -8.279 23.982
ATOM	87	CZ	ARG .	A	8	3.405 -9.541 23.185
ATOM	88	NH1	ARG .	Α	8	2.125 -9.871 23.052
MOTA	89	2HH1	ARG .	Α	8	1.418 -9.321 23.496
ATOM	90	1HH1	ARG .	Α	8	1.869 -10.670 22.508
ATOM	91	NH2	ARG .	Α	8	4.332 -10.286 22.589
ATOM	92	1HH2	ARG .	Α	8	4.062 -11.082 22.048
ATOM	93	2HH2		A	8	5.299 -10.050 22.682
ATOM	94	N	PRO		9	1.990 -2.428 26.938
ATOM	95	CA	PRO .		9	1.001 -1.462 27.440
ATOM	96	C	PRO .		9	-0.365 -1.697 26.821
ATOM	97	Ö	PRO .		9	-0.918 -0.935 26.008
ATOM	98	CB	PRO .		9	1.572 -0.112 27.041
			PRO .		9	2.553 -0.404 25.931
ATOM	99	CG				
ATOM	100	CD	PRO		9	
ATOM	101	N	LEU .		10	-1.028 -2.803 27.227
ATOM	102	H	LEU		10	-0.616 -3.404 27.912
ATOM	103	CA	LEU		10	-2.319 -3.143 26.698
ATOM	104	С	LEU		10	-3.390 -2.565 27.591
MOTA	105	0	LEU		10	-3.336 -2.632 28.831
MOTA	106	CB	LEU	Α	10	-2.451 -4.651 26.709
ATOM	107	CG	LEU	Α	10	-1.483 -5.316 25.756
ATOM	108	CD1	LEU	Α	10	-1.159 -6.740 26.212
ATOM	109	CD2	LEU		10	-2.083 -5.262 24.322
ATOM	110	N	VAL		11	-4.447 -1.952 27.033
ATOM	111	H	VAL		11	-4.507 -1.875 26.038





# Figure 11<sub>C</sub>

MOTA	112	CA	VAL A	11	-5.506	-1.398	27.835
ATOM	113	C	VAL A	11	-6.827	-1.857	27.268
ATOM	114	0	VAL A	11	-6.924	-2.490	26.198
ATOM	115	CB	VAL A	11	-5.420	0.143	27.897
MOTA	116	CG1	VAL A	11	-4.117	0.595	28.551
ATOM	117	CG2	VAL A	11	-5.549	0.787	26.497
ATOM	118	N	THR A	12	-7.954	-1.592	27.978
MOTA	119	H	THR A	12	-7.884	-1.141	28.868
ATOM	120	CA	THR A	12	-9.301	-1.942	27.496
ATOM	121	C	THR A	12	-9.889	-0.726	26.795
			THR A	12	-9.856	0.436	27.247
MOTA	122	O		12	-10.225	-2.385	28.659
ATOM	123	CB	THR A				29.338
ATOM	124	OG1	THR A	12	-9.596	-3.458	
MOTA	125	HG1	THR A	12	-10.170	-3.766	30.096
MOTA	126	CG2	THR A	12	-11.579	-2.895	28.156
MOTA	127	N	ILE A	13	-10.449	-0.932	25.594
MOTA	128	H	ILE A	13	-10.409	-1.841	25.178
MOTA	129	CA	ILE A	13	-11.112	0.133	24.882
MOTA	130	C	ILE A	13	-12.553	-0.292	24.693
MOTA	131	0	ILE A	13	-12.935	-1.469	24.821
MOTA	132	CB	ILE A	13	-10.432	0.364	23.511
ATOM	133	CG1	ILE A	13	-10.466	-0.896	22.628
ATOM	134	CG2	ILE A	13	-8.986	0.806	23.747
ATOM	135	CD1	ILE A	13	-9.755	-0.745	21.294
ATOM	136	N	LYS A	14	-13.470	0.658	24.438
MOTA	137	H	LYS A	14	-13.209	1.622	24.481
ATOM	138	CA	LYS A	14	-14.838	0.330	24.100
ATOM	139	C	LYS A	$\overline{14}$	-15.088	0.877	22.719
ATOM	140	Ö	LYS A	$\frac{14}{14}$	-14.859	2.059	22.375
ATOM	141	СВ	LYS A	14	-15.855	0.916	25.099
ATOM	142	CG	LYS A	14	-17.325	0.518	24.864
ATOM	143	CD	LYS A	14	-18.078	0.146	26.166
ATOM	144	CE	LYS A	14	-18.826	1.342	26.810
ATOM	145	NZ	LYS A	14	-19.316	0.929	28.173
ATOM	146	1HZ	LYS A	14	-19.801	1.693	28.599
	147	3HZ	LYS A	14	-18.536	0.670	28.743
ATOM		2HZ	LYS A	14	-19.936	0.150	28.082
ATOM	148			15	-15.535	0.005	21.798
ATOM	149	N	ILE A	15	-15.806	-0.916	22.078
ATOM	150	H		_		0.347	20.400
ATOM	151	CA	ILE A	15	-15.642	-0.328	19.887
ATOM	152	C	ILE A	15	-16.894		
ATOM	153	0	ILE A	15	-17.115	-1.542	20.041
MOTA	154	CB	ILE A	15	-14.382	-0.132	19.639
ATOM	155	CG1	ILE A	15	-14.478	0.148	18.125
ATOM	156	CG2	ILE A	15	-14.082	-1.623	19.880
ATOM	157	CD1	ILE A	15	-14.237	1.603	17.796
ATOM	158	N	GLY A	16	-17.843	0.435	19.308
ATOM	159	H	GLY A	16	-17.720	1.426	19.260
MOTA	160	CA	GLY A	16	-19.053	-0.143	18.745
MOTA	161	С	GLY A	16	-19.897	-0.817	19.789
ATOM	162	0	GLY A	16	-20.774	-1.668	19.516
ATOM	163	N	GLY A	17	-19.712	-0.493	21.088
ATOM	164	H	GLY A	17	-19.038	0.204	21.334
ATOM	165	CA	GLY A	17	-20.464	-1.126	22.160
ATOM	166	С	GLY A	17	-19.718	-2.335	22.653
MOTA	167	0	GLY A	17	-20.147	-3.098	23.540





# Figure 11D

ATOM	168	N	GLN .	Α	18	-18.507 -2.591 22.121
MOTA	169	H	GLN .	Α	18	-18.059 -1.900 21.554
MOTA	170	CA	GLN .	Α	18	-17.806 -3.830 22.326
MOTA	171	С	GLN .	Α	18	-16.552 -3.549 23.123
ATOM	172	0	GLN .	Α	18	-15.887 -2.508 22.945
ATOM	173	CB	GLN .	Α	18	-17.393 -4.294 20.928
ATOM	174	CG	GLN .	Α	18	-16.911 -5.734 20.788
MOTA	175	CD	GLN .	Α	18	-18.018 -6.728 20.613
ATOM	176	OE1	GLN .	Α	18	-19.131 -6.574 21.152
ATOM	177	NE2	GLN	Α	18	-17.722 -7.773 19.857
ATOM	178	1HE2	GLN .	Α	18	-18.404 -8.484 19.689
ATOM	179	2HE2	GLN .		18	-16.814 -7.860 19.448
ATOM	180	N	LEU .	Α	19	-16.133 -4.397 24.087
ATOM	181	H	LEU .	Α	19	-16.682 -5.202 24.312
ATOM	182	CA	LEU .		19	-14.909 -4.178 24.808
MOTA	183	С	LEU .		19	-13.799 -4.912 24.090
ATOM	184	0	LEU .		19	-13.989 -6.018 23.558
ATOM	185	CB		A	19	-14.982 -4.714 26.254
MOTA	186	CG		Α	19	-15.490 -3.778 27.374
ATOM	187	CD1	LEU		19	-16.392 -2.639 26.856
ATOM	188	CD2	LEU .		19	-16.208 -4.516 28.465
ATOM	189	N		Α	20	-12.603 -4.372 23.978
ATOM	190	Н		Α	20	-12.442 -3.448 24.324
ATOM	191	CA		A	20	-11.507 -5.082 23.365
ATOM	192	C		A	20	-10.266 -4.618 24.062
ATOM	193	Ö		A	20	-10.228 -3.611 24.816
ATOM	194	СВ		A	20	-11.397 -4.798 21.875
ATOM	195	CG		A	20	-12.558 -5.356 21.100
ATOM	196	CD		A	20	-12.537 -4.988 19.615
ATOM	197	CE		A	20	-13.414 -5.958 18.827
ATOM	198	NZ		Α	20	-12.681 -7.208 18.639
ATOM	199	1HZ		A	20	-13.247 -7.852 18.123
ATOM	200	3HZ		A	20	-12.458 -7.601 19.531
ATOM	201	2HZ		Α	20	-11.837 -7.027 18.134
ATOM	202	N	GLU		21	-9.150 -5.357 23.893
ATOM	203	Н		Α	21	-9.185 -6.188 23.338
ATOM	204	CA		Α	21	-7.890 -4.997 24.486
ATOM	205	C	GLU .		21	-7.001 -4.462 23.390
ATOM	206	Ö	GLU		21	-6.970 -4.992 22.258
ATOM .	207	СВ	GLU		21	-7.268 -6.260 25.051
ATOM	208	CG	GLU		21	-5.835 -6.140 25.480
ATOM	209	CD	GLU		21	-5.405 -7.352 26.275
ATOM	210	OE1	GLU		21	-5.624 -7.343 27.508
ATOM	211	OE2	GLU		21	-4.852 -8.309 25.684
ATOM	212	N	ALA		22	-6.239 -3.369 23.595
ATOM	213	H	ALA		22	-6.223 -2.938 24.497
ATOM	214	CA	ALA		22	-5.419 -2.781 22.520
ATOM	215	C	ALA		22	-4.138 -2.255 23.114
ATOM	216	Ö	ALA		22	-3.985 -1.914 24.314
ATOM	217	CB	ALA		22	-6.134 -1.657 21.821
ATOM	218	N	LEU		23	-3.121 -2.091 22.240
ATOM	219	H	LEU		23	-3.279 -2.236 21.263
ATOM	220	CA	LEU		23	-1.797 -1.712 22.640
ATOM	221	C	LEU		23	-1.660 -0.230 22.443
ATOM	222	Ö	LEU		23	-2.020 0.349 21.402
ATOM	223	CB	LEU		23	-0.814 -2.486 21.732
	223	22				0.021 2.100 21.702





## Figure 11E

ATOM	224	CG	LEU A	23	0.705	-2.448	21.991
ATOM	225	CD1	LEU A	23	1.088	-3.400	23.124
ATOM	226	CD2	LEU A	23	1.462	-2.878	20.708
ATOM	227	N	LEU A	24	-1.192	0.530	23.463
ATOM	228	Н	LEU A	24	-1.015	0.110	24.353
ATOM	229	CA	LEU A	24	-0.935	1.952	23.305
ATOM	230	C	LEU A	24	0.403	2.089	22.609
ATOM	231	Ö	LEU A	24	1.471	1.717	23.130
ATOM	232	CB	LEU A	24	-0.921	2.609	24.681
		CG	LEU A	24	-2.220	2.492	25.477
ATOM	233				-2.220	3.291	26.772
ATOM	234	CD1	LEU A	24		3.000	24.691
ATOM	235	CD2	LEU A	24	-3.419		21.397
MOTA	236	N	ASP A	25	0.454	2.590	
MOTA	237	H	ASP A	25	-0.334	3.085	21.032
MOTA	238	CA	ASP A	25	1.642	2.423	20.605
MOTA	239	С	ASP A	25	2.130	3.750	20.059
MOTA	240	0	ASP A	25	1.568	4.320	19.110
MOTA	241	CB	ASP A	25	1.263	1.435	19.486
MOTA	242	CG	ASP A	25	2.428	1.051	18.561
ATOM	243	OD1	ASP A	25	3.546	1.540	18.729
MOTA	244	OD2	ASP A	25	2.164	0.241	17.658
ATOM	245	N	THR A	26	3.203	4.337	20.605
ATOM	246	Н	THR A	26	3.694	3.880	21.346
ATOM	247	CA	THR A	26	3.691	5.652	20.144
ATOM	248	C	THR A	26	4.397	5.583	18.778
ATOM	249	Ö	THR A	26	4.642	6.587	18.079
ATOM	250	СВ	THR A	26	4.596	6.219	21.217
ATOM	251	OG1	THR A	26	5.716	5.324	21.386
ATOM	252	HG1	THR A	26	6.332	5.676	22.091
ATOM	253	CG2	THR A	26	3.878	6.320	22.577
ATOM	254	N	GLY A	27	4.757	4.377	18.298
ATOM	255	H	GLY A	27	4.526	3.550	18.811
ATOM	256	CA	GLY A	27	5.481	4.233	17.040
ATOM	257	C	GLY A	27	4.520	4.190	15.886
	258	0	GLY A	27	4.908	4.242	14.696
ATOM					3.197	4.084	16.117
ATOM	259	N	ALA A	28	2.856	4.091	17.057
ATOM	260	H	ALA A	28		3.955	15.018
ATOM	261	CA	ALA A	28	2.213	5.299	14.750
MOTA	262	C	ALA A	28	1.598		
ATOM	263	0	ALA A	28	1.062	5.982	15.650 15.390
MOTA	264	CB	ALA A	28	1.117	2.980	
ATOM	265	N	ASP A	29	1.503	5.744	13.490
ATOM	266	H	ASP A	29	1.912	5.216	12.746
MOTA	267	CA	ASP A	29	0.810	6.984	13.213
MOTA	268	C	ASP A	29	-0.666	6.724	13.327
MOTA	269	0	ASP A	29	-1.488	7.637	13.568
ATOM	270	CB	ASP A	29	1.009	7.433	11.775
MOTA	271	CG	ASP A	29	2.439	7.882	11.412
ATOM	272	OD1	ASP A	29	3.360	7.856	12.269
MOTA	273	OD2	ASP A	29	2.606	8.253	10.252
ATOM	274	N	ASP A	30	-1.143	5.517	12.990
ATOM	275	H	ASP A	30	-0.508	4.769	12.800
ATOM	276	CA	ASP A	30	-2.579	5.245	12.887
ATOM	277	С	ASP A		-3.057	4.208	13.867
ATOM	278	0	ASP A		-2.284	3.483	14.546
ATOM	279	СВ	ASP A		-2.896	4.758	11.456





# Figure 11F

ATOM	280	CG	ASP A	30	-2.495	5.768	10.425
MOTA	281	OD1	ASP A	30	-3.067	6.871	10.423
ATOM	282	OD2	ASP A	30	-1.596	5.494	9.618
ATOM	283	N	THR A	31	-4.393	4.076	14.002
	284	Н	THR A	31	-5.004	4.700	13.515
ATOM					-5.059	3.062	14.829
ATOM	285	CA	THR A	31			
ATOM	286	С	THR A	31	-5.565	1.967	13.913
MOTA	287	0	THR A	31	-6.223	2.169	12.870
ATOM	288	CB	THR A	31	-6.212	3.725	15.566
ATOM	289	OG1	THR A	31	-5.668	4.667	16.474
ATOM	290	HG1	THR A	31	-6.403	5.122	16.976
ATOM	291	CG2	THR A	31	-7.044	2.702	16.389
	292	N	VAL A	32	-5.187	0.713	14.235
MOTA						0.715	15.063
MOTA	293	H	VAL A	32	-4.649		
ATOM	294	CA	VAL A	32	-5.517	-0.462	13.437
MOTA	295	C	VAL A	32	-6.092	-1.506	14.365
MOTA	296	0	VAL A	32	-5.502	-1.957	15.365
ATOM	297	CB	VAL A	32	-4.260	-1.064	12.757
ATOM	298	CG1	VAL A	32	-4.667	-2.136	11.735
ATOM	299	CG2	VAL A	32	-3.422	0.017	12.032
ATOM	300	N	LEU A	33	-7.352	-1.923	14.119
		H		33	-7.867	-1.523	13.361
ATOM	301		LEU A				
MOTA	302	CA	LEU A	33	-7.982	-2.940	14.929
ATOM	303	C	LEU A	33	-8.174	-4.203	14.107
ATOM	304	0	LEU A	33	-8.268	-4.247	12.853
ATOM	305	CB	LEU A	33	-9.336	-2.477	15.408
ATOM	306	CG	LEU A	33	-9.292	-1.149	16.127
ATOM	307	CD1	LEU A	33	-10.710	-0.747	16.485
ATOM	308	CD2	LEU A	33	-8.348	-1.139	17.347
ATOM	309	N	GLU A	34	-8.296	-5.319	14.782
		H	GLU A	34	-8.244	-5.302	15.780
ATOM	310					-6.551	14.086
ATOM	311	CA	GLU A	34	-8.503		
MOTA	312	C	GLU A	34	-9.909	-6.549	13.510
MOTA	313	0	GLU A	34	-10.808	-5.717	13.795
MOTA	314	CB	GLU A	34	-8.265	-7.750	15.010
ATOM	315	CG	GLU A	34	-9.259	-7.791	16.165
MOTA	316	$^{\rm CD}$	GLU A	34	-8.763	-8.552	17.404
ATOM	317	OE1	GLU A	34	-7.670	-9.193	17.368
ATOM	318	OE2	GLU A	34	-9.482	-8.497	18.407
ATOM	319	N	GLU A	35	-10.152	-7.480	12.568
ATOM	320	H	GLU A	35	-9.485	-8.208	12.407
			GLU A	35	-11.352	-7.466	11.773
ATOM	321	CA					
ATOM	322	C	GLU A	35	-12.631	-7.520	12.571
MOTA	323	0	GLU A	35	-12.814	-8.294	13.528
MOTA	324	CB	GLU A	35	-11.237	-8.536	10.707
ATOM	325	CG	GLU A	35	-9.945	-8.280	9.907
ATOM	326	CD	GLU A	35	-9.872	-8.872	8.486
ATOM	327	OE1	GLU A	35	-10.612	-8.401	7.603
ATOM	328	OE2	GLU A	35	-9.024	-9.776	8.261
	329	N	MET A	36	-13.580	-6.598	12.278
ATOM						-5.967	11.515
ATOM	330	H	MET A	36	-13.439		
ATOM	331	CA	MET A	36	-14.819	-6.495	13.052
ATOM	332	С	MET A	36	-15.826	-5.635	12.271
ATOM	333	0	MET A	36	-15.514	-4.828	11.371
ATOM	334	CB	MET A	36	-14.593	-5.845	14.428
ATOM	335	CG	MET A	36	-14.279	-4.353	14.417





# Figure 11<sub>G</sub>

ATOM	336	SD	MET A	36	-14.251	-3.718	16.099
ATOM	337	CE	MET A	36	-12.487	-3.846	16.409
ATOM	338	N	SER A	37	-17.130	-5.776	12.590
ATOM	339	H	SER A	37	-17.399	-6.431	13.296
ATOM	340	CA	SER A	37	-18.155	-5.005	11.940
		C	SER A	37	-18.286	-3.693	12.657
ATOM	341			37	-18.593	-3.624	13.865
ATOM	342	0	SER A			-5.688	12.032
ATOM	343	CB	SER A	37	-19.506		11.716
ATOM	344	OG	SER A	37	-19.455	-7.054	
MOTA	345	HG	SER A	37	-20.367	-7.457	11.791
ATOM	346	N	LEU A	38	-18.185	-2.569	11.933
MOTA	347	H	LEU A	38	-17.956	-2.625	10.952
MOTA	348	CA	LEU A	38	-18.557	-1.247	12.465
MOTA	349	С	LEU A	38	-19.630	-0.605	11.572
ATOM	350	0	LEU A	38	-19.706	-0.939	10.391
ATOM	351	CB	LEU A	38	-17.315	-0.346	12.588
ATOM	352	CG	LEU A	38	-16.246	-0.818	13.596
ATOM	353	CD1	LEU A	38	-14.998	0.073	13.489
ATOM	354	CD2	LEU A	38	-16.756	-0.787	15.046
ATOM	355	N	PRO A	39	-20.455	0.321	12.108
ATOM	356	CA	PRO A	39	-21.460	1.053	11.339
ATOM	357	C	PRO A	39	-20.824	2.176	10.502
ATOM	358	0	PRO A	39	-19.654	2.519	10.685
ATOM	359	CB	PRO A	39	-22.430	1.607	12.389
		CG	PRO A	39	-21.531	1.845	13.600
ATOM	360			39	-20.539	0.686	13.517
MOTA	361	CD	PRO A		-21.620	2.749	9.586
ATOM	362	N	GLY A	40	-22.569	2.417	9.493
ATOM	363	H	GLY A	40		3.811	8.678
ATOM	364	CA	GLY A	40	-21.203		7.298
MOTA	365	C	GLY A	40	-20.836	3.262	
MOTA	366	0	GLY A	40	-21.405	2.268	6.845
MOTA	367	N	LYS A	41	-19.895	3.945	6.631
MOTA	368	H	LYS A	41	-19.496	4.761	7.071
MOTA	369	$^{\rm CA}$	LYS A	41	-19.323	3.558	5.343
MOTA	370	C	LYS A	41	-17.798	3.757	5.371
ATOM	371	0	LYS A	41	-17.263	4.462	6.229
ATOM	372	CB	LYS A	41	-20.025	4.352	4.224
ATOM	373	CG	LYS A	41	-19.703	3.839	2.810
MOTA	374	CD	LYS A	41	-20.610	4.486	1.757
ATOM	375	CE	LYS A	41	-20.240	3.964	0.366
MOTA	376	NZ	LYS A	41	-21.097	4.552	-0.678
MOTA	377	1HZ	LYS A	41	-20.824	4.189	-1.580
ATOM	378	3HZ	LYS A	41	-20.993	5.556	-0.673
ATOM	379	2HZ	LYS A	41	-22.061	4.311	-0.498
ATOM	380	N	TRP A	42	-17.104	3.091	4.439
ATOM	381	Н	TRP A	42	-17.620	2.548	3.762
ATOM	382	CA	TRP A	42	-15.654	2.932	4.423
		C	TRP A	42	-15.105	2.852	2.994
ATOM	383		TRP A	42	-15.845	2.702	2.021
MOTA	384	0			-15.279	1.675	5.236
MOTA	385	CB	TRP A	42		0.514	5.094
ATOM	386	CG	TRP A	42	-16.214		4.101
ATOM	387	CD1		42	-16.230	-0.402	5.942
ATOM	388	CD2		42	-17.355	0.203	
ATOM	389	NE1		42	-17.297	-1.260	4.281
ATOM	390	HE1		42	-17.504	-2.015	3.644
ATOM	391	CE2	TRP A	42	-18.045	-0.914	5.389





# Figure 11<sub>H</sub>

MOTA	392	CE3	TRP A	42	-17.896	0.792	7.103
MOTA	393	CZ2	TRP A	42	-19.224	-1.421	5.959
ATOM	394	CZ3	TRP A	42	-19.077	0.298	7.675
ATOM	395	CH2	TRP A	42	-19.741	-0.806	7.112
ATOM	396	N	LYS A	43	-13.771	2.932	2.911
ATOM	397	H	LYS A	43	-13.260	3.058	3.773
ATOM	398	CA	LYS A	43	-12.951	2.802	1.713
ATOM	399	C	LYS A	43	-11.773	1.859	2.012
ATOM	400	0	LYS A	43	-11.359	1.760	3.166
		CB		43	-12.451	4.193	1.270
ATOM	401				-11.724	4.979	2.383
ATOM	402	CG	LYS A	43		6.267	1.873
ATOM	403	CD	LYS A	43	-11.060		
ATOM	404	CE	LYS A	43	-9.784	6.001	1.065
MOTA	405	NZ	LYS A	43	-8.700	5.458	1.903
MOTA	406	1HZ	LYS A	43	-7.876	5.315	1.338
MOTA	407	3HZ	LYS A	43	-8.993	4.576	2.300
ATOM	408	2HZ	LYS A	43	-8.493	6.108	2.647
ATOM	409	N	PRO A	44	-11.177	1.197	1.004
ATOM	410	CA	PRO A	44	-9.947	0.435	1.187
ATOM	411	C	PRO A	44	-8.760	1.392	1.379
ATOM	412	0	PRO A	44	-8.711	2.434	0.720
ATOM	413	CB	PRO A	44	-9.808	-0.393	-0.095
ATOM	414	CG	PRO A	44	-10.501	0.458	-1.159
ATOM	415	CD	PRO A	44	-11.630	1.132	-0.380
ATOM	416	N	LYS A	45	-7.790	1.030	2.240
ATOM	417	H	LYS A	45	-7.912	0.227	2.824
ATOM	418	CA	LYS A	45	-6.547	1.747	2.314
ATOM	419	C	LYS A	45	-5.493	0.683	2.507
ATOM	420	0	LYS A	45	-5.780	-0.470	2.869
	421		LYS A	45	-6.594	2.699	3.524
ATOM		CB	LYS A	45	-5.463	3.744	3.609
ATOM	422	CG	LYS A	45	-5.340	4.289	5.052
ATOM	423	CD		45	-4.262	5.383	5.204
MOTA	424	CE	LYS A		-2.907	4.911	4.916
ATOM	425	NZ	LYS A	45	-2.260	5.664	5.032
ATOM	426	1HZ	LYS A	45		4.577	3.975
ATOM	427	3HZ	LYS A	45	-2.864 -2.672	4.169	5.544
ATOM	428	2HZ	LYS A	45			2.193
ATOM	429	N	MET A	46	-4.224	0.949	
ATOM	430	H	MET A	46	-3.998	1.805	1.728
ATOM	431	CA	MET A	46	-3.157	0.027	2.509
ATOM	432	C	MET A	46	-2.417	0.701	3.627
ATOM	433	0	MET A	46	-2.259	1.937	3.634
ATOM	434	CB	MET A	46	-2.166	-0.088	1.379
ATOM	435	CG	MET A	46	-2.782	-0.366	0.053
ATOM	436	SD	MET A		-3.076	-2.108	-0.118
MOTA	437	CE	MET A		-1.417	-2.652	-0.186
ATOM	438	N	ILE A		-1.827	-0.016	4.586
ATOM	439	H	ILE A	47	-2.010	-0.997	4.655
MOTA	440	CA	ILE A	47	-0.922	0.586	5.539
MOTA	441	C	ILE A	47	0.233	-0.372	5.654
MOTA	442	0	ILE A	47	0.135	-1.584	5.356
ATOM	443	CB	ILE A	47	-1.550	0.836	6.923
MOTA	444	CG1	ILE A	47	-2.459	-0.301	7.354
ATOM	445	CG2	ILE A	47	-2.248	2.164	6.995
ATOM	446	CD1	ILE A		-1.724	-1.336	8.111
MOTA	447	N	GLY A		1.420	0.089	6.043





## Figure 111

ATOM	448	H	GLY A	48	1.509	1.040	6.339
ATOM	449	CA	GLY A	48	2.584	-0.753	6.048
ATOM	450	С	GLY A	48	3.280	-0.657	7.376
ATOM	451	0	GLY A	48	3.050	0.190	8.265
MOTA	452	N	GLY A	49	4.197	-1.617	7.603
MOTA	453	Н	GLY A	49	4.375	-2.308	6.902
ATOM	454	CA	GLY A	49	4.936	-1.684	8.828
ATOM	455	C	GLY A	49	6.105	-2.589	8.533
MOTA	456	Ö	GLY A	49	6.482	-2.807	7.370
MOTA	457	N	ILE A	50	6.761	-3.173	9.552
ATOM	458	H	ILE A	50	6.552	-2.908	10.493
ATOM	459	CA	ILE A	50	7.772	-4.184	9.344
	460	CA	ILE A	50	7.148	-5.317	8.566
MOTA MOTA		0		50	5.981	-5.734	8.772
	461		ILE A				
ATOM	462	CB	ILE A	50	8.258	-4.686	10.722
MOTA	463	CG1	ILE A	50	9.257	-3.714	11.382
ATOM	464	CG2	ILE A	50	8.813	-6.134	10.693
ATOM	465	CD1	ILE A	50	10.580	-3.498	10.628
MOTA	466	N	GLY A	51	7.847	-5.891	7.596
MOTA	467	H	GLY A	51	8.772	-5.569	7.395
ATOM	468	CA	GLY A	51	7.265	-6.966	6.850
ATOM	469	C	GLY A	51	6.519	-6.559	5.591
MOTA	470	0	GLY A	51	6.430	-7.318	4.634
ATOM	471	N	GLY A	52	5.886	-5.375	5.517
ATOM	472	H	GLY A	52	5.990	-4.710	6.257
ATOM	473	CA	GLY A	52	5.108	-5.227	4.320
MOTA	474	С	GLY A	52	3.832	-4.415	4.516
ATOM	475	0	GLY A	52	3.654	-3.624	5.467
ATOM	476	N	PHE A	53	2.886	-4.518	3.559
ATOM	477	Н	PHE A	53	3.013	-5.161	2.804
MOTA	478	CA	PHE A	53	1.653	-3.720	3.566
ATOM	479	C	PHE A	53	0.494	-4.651	3.783
ATOM	480	Õ	PHE A	53	0.448	-5.816	3.336
ATOM	481	CB	PHE A	53	1.424	-3.022	2.221
ATOM	482	CG	PHE A	53	2.363	-1.896	2.008
ATOM	483	CD1	PHE A	53	3.615	-2.135	1.447
ATOM	484	CD2	PHE A	53	2.011	-0.608	2.414
ATOM	485	CE1	PHE A	53	4.514	-1.087	1.275
ATOM	486	CE2	PHE A	53	2.925	0.446	2.237
ATOM	487	CZ	PHE A	53	4.172	0.202	1.668
ATOM	488	N	ILE A	54	-0.554	-4.173	4.439
			ILE A	54	-0.491	-3.285	4.895
ATOM	489	H			-1.789	-4.911	
ATOM	490	CA	ILE A	54			4.509
MOTA	491	C	ILE A	54	-2.903	-3.995	4.033
ATOM	492	O	ILE A	54	-2.751	-2.770	3.855
ATOM	493	CB	ILE A	54	-2.034	-5.535	5.904
ATOM	494	CG1	ILE A	54	-2.343	-4.481	6.988
ATOM	495	CG2	ILE A	54	-0.799	-6.318	6.314
ATOM	496	CD1	ILE A	54	-3.010	-5.089	8.246
ATOM	497	N	LYS A	55	-4.029	-4.577	3.560
ATOM	498	H	LYS A	55	-4.084	-5.574	3.501
MOTA	499	CA	LYS A	55	-5.177	-3.798	3.129
ATOM	500	С	LYS A	55	-6.115	-3.726	4.300
MOTA	501	0	LYS A	55	-6.422	-4.707	5.023
MOTA	502	CB	LYS A	55	-5.928	-4.461	1.938
MOTA	503	CG	LYS A	55	-6.853	-3.547	1.106





# Figure $11_{\rm J}$

ATOM	504	$^{\rm CD}$	LYS	Α	55	-8.267	-3.332	1.714
MOTA	505	CE	LYS	Α	55	-9.303	-4.392	1.301
ATOM	506	NZ	LYS	Α	55	-10.521	-4.453	2.192
ATOM	507	1HZ	LYS	Α	55	-11.142	-5.162	1.859
ATOM	508	3HZ	LYS	Α	55	-10.987	-3.569	2.180
MOTA	509	2HZ	LYS	Α	55	-10.240	-4.669	3.127
MOTA	510	N	VAL	Α	56	-6.599	-2.509	4.619
MOTA	511	H	VAL		56	-6.337	-1.713	4.073
ATOM	512	CA	VAL	Α	56	-7.494	-2.311	5.735
ATOM	513	C	VAL		56	-8.711	-1.584	5.236
MOTA	514	0	VAL		56	-8.767	-1.029	4.114
ATOM	515	CB	VAL		56	-6.759	-1.475	6.812
ATOM	516	CG1	VAL		56	-5.569	-2.209	7.385
ATOM	517	CG2	VAL		56	-6.287	-0.108	6.268
ATOM	518	N	ARG		57	-9.784	-1.539	6.005
ATOM	519	H	ARG		57	-9.835	-2.117	6.819
ATOM	520	CA	ARG		57	-10.855	-0.648	5.638
ATOM	521	C	ARG		57	-10.738	0.534	6.554
ATOM	522	0	ARG		57	-10.558	0.449	7.789
ATOM	523	CB	ARG		57	-12.219	-1.271	5.835 4.952
ATOM	524	CG	ARG		57	-12.480	-2.452	5.195
ATOM	525	CD	ARG		57 57	-13.834 -14.122	-3.051 -4.137	4.270
ATOM	526	NE	ARG ARG		57	-14.122	-4.137 -4.347	3.568
ATOM	527	HE CZ	ARG		57 57	-15.243	-4.851	4.324
ATOM	528 529	NH1	ARG		5 <i>7</i>	-16.175	-4.624	5.243
ATOM ATOM	530	2HH1	ARG		5 <i>7</i>	-16.044	-3.899	5.920
ATOM	531	1HH1	ARG		57	-17.008	-5.178	5.258
ATOM	532	NH2	ARG		5 <i>7</i>	-15.433	-5.822	3.434
ATOM	533	1HH2		A	57	-16.270	-6.368	3.461
ATOM	534	2HH2	ARG		57	-14.738	-6.006	2.738
ATOM	535	N		Α	58	-10.881	1.741	6.036
ATOM	536	Н		A	58	-11.030	1.844	5.053
ATOM	537	CA		A	58	-10.830	2.922	6.839
ATOM	538	C	GLN		58	-12.231	3.342	7.205
ATOM	539	0	GLN		58	-13.106	3.608	6.359
ATOM	540	CB	GLN	Α	58	-10.208	4.038	6.030
ATOM	541	CG	GLN	Α	58	-10.055	5.293	6.817
ATOM	542	CD	GLN	Α	58	-9.632	6.411	5.927
ATOM	543	OE1	GLN	Α	58	-10.379	7.334	5.662
ATOM	544	NE2	GLN	Α	58	-8.412	6.303	5.437
ATOM	545	1HE2	$\operatorname{GLN}$	Α	58	-8.047	7.009	4.830
MOTA	546	2HE2	GLN		58	-7.843	5.514	5.668
ATOM	547	N	TYR		59	-12.527	3.516	8.509
ATOM	548	H	TYR		59	-11.877	3.219	9.209
ATOM	549	CA	TYR		59	-13.769	4.125	8.933
ATOM	550	C	TYR		59	-13.411	5.452	9.565
ATOM	551	0	TYR		59	-12.416	5.592	10.310
ATOM	552	CB	TYR		59	-14.517	3.252	9.957
ATOM	553	CG	TYR		59	-14.287	1.770	9.723
ATOM	554	CD1	TYR		59	-13.007	1.269	9.457
ATOM	555	CD2	TYR		59	-15.346	0.865	9.766
ATOM	556	CE1	TYR		59	-12.797	-0.092	9.240
ATOM	557	CE2	TYR		59	-15.148	-0.494	9.551
ATOM	558	CZ	TYR		59 50	-13.873	-0.972	9.287
ATOM	559	ОН	TYR	А	59	-13.721	-2.311	9.079





# Figure $11_{\!K}$

ATOM	560	нн	TYR A	59	-14.606	-2.771	9.154
ATOM	561	N	ASP A	60	-14.151	6.542	9.300
ATOM	562	H	ASP A	60	-14.954	6.464	8.709
ATOM	563	CA	ASP A	60	-13.822	7.836	9.846
	564	C	ASP A	60	-14.782	8.226	10.947
ATOM			ASP A	60	-15.941	7.765	11.053
ATOM	565	O				8.942	8.769
MOTA	566	CB	ASP A	60	-13.861		7.725
MOTA	567	CG	ASP A	60	-12.735	8.830	
ATOM	568	OD1	ASP A	60	-11.545	8.874	8.075
ATOM	569	OD2	ASP A	60	-13.060	8.702	6.544
MOTA	570	N	GLN A	61	-14.339	9.154	11.833
ATOM	571	H	GLN A	61	-13.385	9.451	11.804
MOTA	572	CA	GLN A	61	-15.151	9.804	12.885
ATOM	573	С	GLN A	61	-15.839	8.803	13.802
ATOM	574	0	GLN A	61	-17.008	8.893	14.229
ATOM	575	CB	GLN A	61	-16.097	10.908	12.338
ATOM	576	CG	GLN A	61	-16.239	12.133	13.262
ATOM	577	CD	GLN A	61	-16.910	13.366	12.629
	578	OE1	GLN A	61	-16.509	13.854	11.586
MOTA		NE2	GLN A	61	-17.937	13.887	13.292
ATOM	579			61	-18.416	14.689	12.934
ATOM	580	1HE2	GLN A			13.482	14.155
ATOM	581	2HE2	GLN A	61	-18.239		14.175
MOTA	582	N	ILE A	62	-15.060	7.760	
MOTA	583	H	ILE A	62	-14.111	7.714	13.862
MOTA	584	CA	ILE A	62	-15.557	6.705	15.015
ATOM	585	С	ILE A	62	-15.251	7.057	16.447
ATOM	586	0	ILE A	62	-14.198	7.613	16.837
MOTA	587	CB	ILE A	62	-14.829	5.397	14.653
MOTA	588	CG1	ILE A	62	-15.253	4.966	13.258
MOTA	589	CG2	ILE A	62	-15.106	4.271	15.675
ATOM	590	CD1	ILE A	62	-16.779	4.788	13.116
ATOM	591	N	LEU A	63	-16.242	6.807	17.320
ATOM	592	H	LEU A	63	-17.089	6.383	17.000
ATOM	593	CA	LEU A	63	-16.127	7.131	18.719
MOTA	594	C	LEU A	63	-15.518	5.942	19.425
ATOM	595	Ö	LEU A	63	-15.869	4.753	19.269
ATOM	596	CB	LEU A	63	-17.512	7.428	19.282
ATOM	597	CG	LEU A	63	-17.660	7.598	20.813
	598		LEU A		-16.711	8.632	21.404
ATOM					-19.089	7.963	21.201
ATOM	599	CD2	LEU A		-14.511	6.211	20.219
ATOM	600	N	ILE A				20.305
ATOM	601	H	ILE A		-14.185	7.153	
ATOM	602	CA	ILE A		-13.862	5.178	20.972
ATOM	603	C	ILE A		-13.529	5.744	22.325
ATOM	604	0	ILE A		-13.396	6.959	22.602
MOTA	605	CB	ILE A		-12.618	4.716	20.231
ATOM	606	CG1	ILE A		-11.925	3.573	20.949
ATOM	607	CG2	ILE A	64	-11.690	5.865	19.950
MOTA	608	CD1	ILE A		-10.905	2.888	20.062
ATOM	609	N	GLU A	65	-13.396	4.815	23.294
ATOM	610	Н	GLU A	65	-13.443	3.844	23.059
ATOM	611	CA	GLU A		-13.186	5.174	24.670
MOTA	612	C	GLU A		-12.024	4.360	25.165
ATOM	613	Ö	GLU A		-11.943	3.112	25.056
ATOM	614	СВ	GLU A		-14.459	4.823	25.405
ATOM	615	CG	GLU A		-14.739	5.610	26.646
AION	010		OLO A		± 4 . , 5	2.323	





# Figure 11L

				- 3			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	61789012345678901234567890123456789012345666666666666666666666666666666666666	CD 1 OE 1 OE 2 N H C C O C G N H C C O N H C C O C C N H C C O C C C C C C C N H C C O C C N H C C C N N H C C O C C C C N C C C N C C C C C C C C	GLUU AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA	66666666666666666666666666666666666666	-16.131 -17.090 -16.269 -10.971 -11.009 -9.762 -9.571 -9.422 -8.600 -8.838 -7.231 -9.9.698 -10.673 -10.393 -8.251 -7.170 -11.877 -12.125 -12.788 -12.788 -12.1838 -11.504 -11.305 -11.838 -9.317 -9.831 -9.317 -9.688 -9.317 -9.688 -10.645 -11.516 -9.317 -9.688 -10.516 -9.317 -11.505 -12.346 -11.587 -14.645 -15.837 -14.645 -15.837 -17.105 -18.293 -18.303 -19.563 -19.563 -19.563 -19.563	5.37878 5.7088 6.0024.3174.582 4.573074.6694.3284.9824.9842 5.740394.9842 5.740394.9842 6.80792864 7.74286423 7.742864	
ATOM ATOM ATOM	665 666 667	N H CA	ALA A ALA A ALA A	71 71 71	-12.323 -12.813 -11.616	9.485 8.625 10.044	24.663 22.446 22.305 21.333 20.171
ATOM ATOM ATOM ATOM	668 669 670 671	C O CB N	ALA A ALA A ALA A ILE A	71 71 71 72	-12.529 -13.351 -10.292 -12.559	9.795 8.850 9.358 10.685	20.171 20.146 21.143 19.149





## Figure 11M

3 moss	600			_		70.00	11 515	10 000
ATOM	672	H	ILE .		72	-12.006	11.517	19.200
MOTA	673	CA	ILE .	Α	72	-13.376	10.474	17.963
ATOM	674	С	ILE .	Α	72	-12.480	10.662	16.771
ATOM	675	0	ILE .	Α	72	-11.858	11.720	16.550
ATOM	676	CB		Α	72	-14.541	11.464	17.882
ATOM	677	CG1		A	72	-15.306	11.455	19.196
ATOM	678	CG2		A	72	-15.429	11.203	16.651
MOTA	679	CD1		A	72	-16.446	12.415	19.176
MOTA	680	N	GLY .	Α	73	-12.252	9.633	15.958
ATOM	681	H	GLY .	Α	73	-12.778	8.789	16.067
ATOM	682	CA	GLY .		73	-11.253	9.755	14.938
ATOM	683	C	GLY .		73	-11.283	8.554	14.034
ATOM						-12.211	7.706	
	684	0	GLY .		73			14.006
ATOM	685	N	THR .		74	-10.247	8.428	13.182
ATOM	686	H	THR .	A	74	-9.471	9.055	13.250
ATOM	687	CA	THR .	Α	74	-10.201	7.416	12.158
ATOM	688	С	THR .	Α	74	-9.674	6.134	12.760
ATOM	689	0		Α	74	-8.670	6.034	13.497
ATOM	690	CB		A	74	-9.298	7.895	11.048
ATOM	691							
		OG1		A	74	-9.910	9.019	10.441
ATOM	692	HG1	THR .		74	-9.335	9.362	9.698
ATOM	693	CG2	THR .	A	74	-9.088	6.823	9.946
ATOM	694	N	VAL .	A	75	-10.318	5.027	12.327
ATOM	695	H	VAL .	A	75	-11.066	5.114	11.669
ATOM	696	CA		Α	75	-9.968	3.717	12.778
ATOM	697	C	VAL		75	-9.906	2.843	11.551
ATOM	698	0	VAL		75	-10.803	2.807	
								10.681
ATOM	699	CB	VAL Z		75	-11.044	3.250	13.737
MOTA	700	CG1	VAL 2		75	-11.021	1.721	13.943
ATOM	701	CG2	VAL A	Α	75	-10.915	4.019	15.034
ATOM	702	N	LEU Z	Α	76	-8.768	2.139	11.366
ATOM	703	H		Α	76	-8.002	2.260	11.998
ATOM	704	CA		A	76	-8.566	1.183	10.276
ATOM	705	C		A	76	-8.848	-0.211	10.808
ATOM	706	0		A	76	-8.514	-0.582	11.958
MOTA	707	CB		A	76	-7.103	1.270	9.798
ATOM	708	CG	LEU Z	A	76	-6.608	2.684	9.443
ATOM	709	CD1	LEU Z	Α	76	-5.151	2.645	9.087
ATOM	710	CD2	LEU Z	Α	76	-7.396	3.302	8.296
ATOM	711	N	VAL Z	Α	77	-9.569	-1.062	10.042
ATOM	712	H	VAL Z		77	-9.894	-0.766	9.144
ATOM	713	CA		A	77	-9.899	-2.428	10.485
MOTA	714	C	VAL A		77	-9.298	-3.412	9.482
ATOM	715	0	VAL A		77	-9.450	-3.300	8.253
MOTA	716	CB	VAL A	A	77	-11.436	-2.592	10.506
MOTA	717	CG1	VAL A	Α	77	-11.830	-4.021	10.682
ATOM	718	CG2	VAL Z	Α	77	-12.072	-1.765	11.634
ATOM	719	N	GLY Z		78	-8.560	-4.402	9.928
ATOM	720	H	GLY A		78	-8.445	-4.530	10.913
ATOM								
	721	CA	GLY A		78	-7.930	-5.285	8.987
ATOM	722	C	GLY A		78	-7.228	-6.380	9.732
ATOM	723	0	GLY A	A	78	-7.292	-6.524	10.970
ATOM	724	N	PRO A	Ą	79	-6.512	-7.271	9.003
ATOM	725	CA	PRO A	A	79	-5.880	-8.467	9.602
ATOM	726	С		Α	79	-4.599	-8.107	10.340
ATOM	727	Ö	PRO A		79	-3.449	-8.489	10.032
	. 4.	_	_ 1.CO I	-		3,442	0.107	10.002





# Figure 11N

MOTA	728	CB	PRO A	A 79	-5.613	-9.379	8.400
MOTA	729	CG	PRO A		-5.529	-8.416	7.210
ATOM	730	CD	PRO A		-6.415	-7.225	7.537
MOTA	731	N	THR A		-4.759	-7.304	11.408
ATOM	732	H	THR A		-5.664	-6.935	11.619
ATOM	733	CA	THR A		-3.658	-6.957	12.263
ATOM	734	C	THR A		-3.490	-8.075	13.308
ATOM	735	0	THR A		-4.447	-8.642	13.857
ATOM	736	CB	THR A		-3.868	-5.572	12.927
ATOM	737	OG1	THR F		-2.770	-5.303	
ATOM	738	HG1	THR F				13.787
ATOM					-2.889	-4.412	14.225
	739	CG2	THR A		-5.210	-5.464	13.678
ATOM	740	N	PRO A		-2.243	-8.496	13.589
ATOM	741	CA	PRO P		-1.986	-9.476	14.660
ATOM	742	C	PRO P		-2.499	-8.952	16.001
ATOM	743	0	PRO A		-2.944	-9.720	16.866
MOTA	744	CB	PRO A		-0.444	-9.549	14.732
ATOM	745	CG	PRO A		0.069	-8.951	13.429
ATOM	746	$^{\mathrm{CD}}$	PRO A		-1.029	-8.105	12.842
ATOM	747	N	VAL A	82	-2.474	-7.621	16.276
ATOM	748	H	VAL A	82	-2.180	-6.975	15.571
ATOM	749	CA	VAL A	82	-2.869	-7.091	17.591
ATOM	750	С	VAL A	82	-3.605	-5.761	17.379
MOTA	751	0	VAL A	82	-3.349	-5.004	16.429
ATOM	752	CB	VAL A	82	-1.595	-6.858	18.443
ATOM	753	CG1	VAL A		-0.650	-5.824	17.803
ATOM	754	CG2	VAL A		-1.907	-6.418	19.890
ATOM	755	N	ASN A		-4.548	-5.371	18.260
ATOM	756	H	ASN A		-4.810	-5.981	19.007
ATOM	757	CA	ASN A		-5.181	-4.067	18.123
ATOM	758	C	ASN A		-4.195	-3.019	18.565
ATOM	759	Ö	ASN A		-3.605	-3.064	19.665
ATOM	760	CB	ASN A		-6.436	-3.942	18.982
ATOM	761	CG	ASN A		-7.502	-4.930	18.631
ATOM	762	OD1	ASN A		-7.899	-5.049	17.488
ATOM	763	ND2	ASN A		-7.980	-5.662	19.628
ATOM	764	2HD2	ASN A		-8.695	-6.341	19.459
ATOM	765	1HD2	ASN A		-7.630	-5.541	20.557
ATOM	766	N	ILE A		-4.007	-1.951	17.770
ATOM	767	H	ILE A		-4.583	-1.827	16.962
ATOM	768	CA	ILE A			-0.954	
ATOM	769	C			-2.993		18.032
ATOM			ILE A		-3.679	0.387	18.114
ATOM	770	O	ILE A		-4.460	0.797	17.240
	771	CB	ILE A		-2.021	-0.922	16.833
ATOM	772	CG1	ILE A		-1.162	-2.150	16.859
ATOM	773	CG2	ILE A		-1.219	0.387	16.747
ATOM	774	CD1	ILE A		-0.375	-2.360	15.579
ATOM	775	N	ILE A		-3.471	1.155	19.203
ATOM	776	H	ILE A		-2.972	0.781	19.985
ATOM	777	CA	ILE A		-3.951	2.518	19.281
ATOM	778	C	ILE A		-2.784	3.425	18.949
ATOM	779	0	ILE A		-1.767	3.515	19.663
ATOM	780	CB	ILE A		-4.522	2.825	20.676
ATOM	781	CG1	ILE A		-5.673	1.865	21.050
ATOM	782	CG2	ILE A		-5.000	4.274	20.716
ATOM	783	CD1	ILE A	85	-6.828	1.808	20.059





# Figure 110

ATOM	784	N	GLY A	A 8	6	-2.	820	4	.123	17.	792
ATOM	785	H	GLY A	A 8	6	-3.	637	4	.087		217
ATOM	786	CA	GLY A	A 8	6	-1.	690		.936		351
ATOM	787	C	GLY A	A 8	6	-1.	831		.393		704
ATOM	788	0	GLY A	A 8	6	-2.	760		.864		390
ATOM	789	N	ARG A	A. 8	7	-0.	881		.229		230
ATOM	790	H	ARG A	A 8	7	-0.	204	6	.890		577
MOTA	791	CA	ARG A	A. 8	7		810		.623		643
ATOM	792	С	ARG A	A 8	37		027		.445		277
ATOM	793	0	ARG A	A. 8	37	-2.	365		.430		963
MOTA	794	CB	ARG A	A. 8	37	0.	450		.275		057
ATOM	795	CG	ARG A	A 8	17		735		.496		205
ATOM	796	CD	ARG A	A. 8	37	2.	762		.916		207
MOTA	79 <b>7</b>	NE	ARG A	A. 8	37		875		.961		117
MOTA	798	$_{ m HE}$	ARG A	A 8	37		.035		.353		895
MOTA	799	CZ	ARG A		37		660		.893		035
ATOM	800	NH1	ARG A		37		.463		.675		975
MOTA	801	2HH1	ARG A		37		.712		.335		974
MOTA	802	1HH1	ARG A		37		.066		.602		181
ATOM	803	NH2	ARG A		37		. 656		.019		023
MOTA	804	1HH2	ARG 2		37		.254		.953		224
MOTA	805	2HH2	ARG 2		37		.810		.426		813
ATOM	806	N	ASN A		88		.780		.120		214
MOTA	807	H	ASN .		88		.504		.361		625
MOTA	808	CA	ASN .		38		.015		.860		.890
MOTA	809	C	ASN 2		88		. 963		.921		069
MOTA	810	0	ASN A		38		.613		.954		345
ATOM	811	CB	ASN .		38		.712		.315		617
MOTA	812	CG			38		.475		.001		827
MOTA	813	OD1			38		.922		.996		.245
MOTA	814	ND2			38		.758		.998		.506
MOTA	815	2HD2	ASN .		38		.306		.169		622
ATOM	816	1HD2			38		.190		.824		.145
ATOM	817	N	LEU .		39		.130		.847		.848
MOTA	818	H	LEU .		39		.637		.002		.640
ATOM	819	CA			39		.024		.865		.013
ATOM	820	С			39		.275		.091		.309
ATOM	821	0			39		.834		.632		.283
MOTA	822	CB	LEU .		39		.840		.592		.140
MOTA	823	CG	LEU .		39		.759		.355		.957
ATOM	824	CD1	LEU		39		.369		.980		.088
ATOM	825	CD2	LEU		39		.817		.457		.801
ATOM	826	N	LEU		90		.983		.745		.428
ATOM	827	H	LEU		90		.525		.274		.674
ATOM	828	CA	LEU		90		.242		.057		.664
MOTA	829	С	LEU		90		.155		.555		.932
MOTA	830	0	LEU		90		.202		.020		.092
ATOM	831	CB	LEU		90		.817		.453		.661
ATOM	832	CG	LEU		90		.766		.914		.587
ATOM	833	CD1	LEU		90		.343		.494		.396
ATOM	834	CD2	LEU		90		.339		.230		.812
ATOM	835	N	THR		91		.031		.407		.926
ATOM	836	H	THR		91		.982		.063		.988
ATOM	837	CA	THR		91		.964		.834		.155
ATOM	838	C	THR		91		.309		.331		.635
MOTA	839	0	THR	A 9	91	-4	.422	14	.315	22	.398





# Figure 11<sub>P</sub>

ATOM	840	CB	THR A	91	-2.555	13.543	19.848
ATOM	841	OG1	THR A		-3.459	13.214	18.802
ATOM	842	HG1	THR A		-3.188	13.677	17.958
ATOM	843	CG2	THR A		-1.153	13.122	19.395
	844	N	GLN A		-5.435	12.704	21.258
MOTA			GLN A		-5.379	11.892	20.677
ATOM	845	H			-6.763	13.186	21.682
ATOM	846	CA	GLN A			12.975	23.153
MOTA	847	C	GLN A		-6.942		
MOTA	848	0	GLN A		-7.554	13.797	23.871
ATOM	849	CB	GLN A		-7.890	12.479	20.964
MOTA	850	CG	GLN A		-7.937	12.862	19.517
ATOM	851	CD	GLN A		-9.251	12.515	18.886
ATOM	852	OE1	GLN A	92	-10.270	12.424	19.546
MOTA	853	NE2	GLN A	A 92	-9.202	12.323	17.588
ATOM	854	1HE2	GLN A	92	-10.031	12.087	17.080
MOTA	855	2HE2	GLN A	92	-8.336	12.411	17.097
ATOM	856	N	ILE A	A 93	-6.472	11.846	23.721
ATOM	857	Н	ILE A		-6.014	11.160	23.155
ATOM	858	CA	ILE A		-6.608	11.578	25.165
ATOM	859	C	ILE A		-5.472	12.189	25.948
ATOM	860	Õ	ILE A		-5.342	12.031	27.171
ATOM	861	CB	ILE A		-6.820	10.073	25.484
ATOM	862	CG1	ILE A		-5.536	9.221	25.286
	863	CG2	ILE A		-8.022	9.486	24.735
ATOM		CD1	ILE A		-5.754	7.740	25.693
ATOM	864				-4.594	12.993	25.330
ATOM	865	N	GLY A		-4.617	13.079	24.334
ATOM	866	H	GLY A		-3.613	13.742	26.063
ATOM	867	CA	GLY A		-2.448	12.895	26.512
ATOM	868	C	GLY A				27.519
ATOM	869	0	GLY A		-1.764	13.158	25.797
ATOM	870	N	CYS A		-2.117	11.849	
ATOM	871	H	CYS A		-2.619	11.644	24.957
ATOM	872	CA	CYS A		-1.036	10.994	26.214
ATOM	873	С	CYS A		0.362	11.566	25.925
MOTA	874	0	CYS A		0.588	12.254	24.907
ATOM	875	CB	CYS A		-1.260	9.655	25.550
ATOM	876	SG	CYS 7		-0.254	8.307	26.125
ATOM	877	N	THR A		1.346	11.297	26.803
ATOM	878	H	THR A	A 96	1.135	10.738	27.618
MOTA	879	CA	THR A	A 96	2.728	11.779	26.664
ATOM	880	С	THR A	A 96	3.729	10.784	27.264
ATOM	881	0	THR A	A 96	3.498	10.249	28.345
ATOM	882	CB	THR I	A 96	2.925	13.154	27.346
ATOM	883	OG1	THR A		2.594	13.109	28.721
ATOM	884	HG1	THR Z		2.784	13.966	29.109
ATOM	885	CG2	THR		2.139	14.300	26.698
ATOM	886	N	LEU Z		4.882	10.603	26.599
ATOM	887	H	LEU A		5.016	11.071	25.714
		CA	LEU		6.040	9.910	27.166
ATOM	888	CA	LEU		6.751	10.824	28.175
ATOM	889				6.705	12.046	28.044
ATOM	890	O	LEU		7.013	9.497	26.049
ATOM	891	CB	LEU .				25.065
ATOM	892	CG	LEU .		6.452	8.449	
ATOM	893	CD1			7.360	8.355	23.828
ATOM	894	CD2	LEU .		6.345	7.065	25.724 29.175
ATOM	895	N	ASN .	A 98	7.412	10.221	49.113





# Figure 11<sup>Q</sup>

ATOM	896	Н	ASN A	A	98	7.41	3	9.212	29.205
ATOM	897	CA	ASN A	Ą	98	8.06	-	10.897	30.292
ATOM	898	C	ASN A	A	98	9.22	0	10.029	30.800
ATOM	899	0	ASN A	A	98	8.99	5	9.079	31.550
ATOM	900	CB	ASN A		98	7.05	7	11.177	31.423
ATOM	901	CG	ASN A		98	6.08	4	12.305	31.083
ATOM	902	OD1	ASN A		98	4.98		12.062	30.594
ATOM	903	ND2		Ā	98	6.49		13.549	31.342
ATOM	904	2HD2		Ā	98	5.88		14.331	31.136
ATOM	905	1HD2		A	98	7.40		13.707	31.742
ATOM	906	N		A	99	10.45		10.369	30.389
ATOM	907	H	LEU A		99	10.54		11.177	29.792
	908	CA		A	99	11.67		9.620	30.666
MOTA	909	CA		A.	99	12.71		10.437	31.454
ATOM				A.	99	12.48		11.652	31.651
MOTA	910	O		A.	99	12.23		8.989	29.369
ATOM	911	CB				12.83		9.873	28.248
MOTA	912	CG		A	99	11.87		10.947	27.705
MOTA	913	CD1		A	99				28.623
ATOM	914	CD2		A	99	14.18		10.505	31.869
ATOM	915	TXO	LEU A	A	99	13.71	6	9.819	31.009
TER				_	_	10.60	_	14 007	30.106
MOTA	916	N		В	1	12.60		14.237	
MOTA	917	CA		В	1	11.84		15.268	29.363
MOTA	918	C		В	1	10.43		14.773	29.138
MOTA	919	0		В	1	10.05		13.695	29.618
ATOM	920	CB	PRO :		1	12.62		15.412	28.035
MOTA	921	CG		В	1	13.81		14.470	28.131
ATOM	922	$^{\rm CD}$	PRO	В	1	13.96		14.227	29.603
ATOM	923	1H	PRO	В	1	12.17		13.343	29.964
ATOM	924	2H	PRO	В	1	12.59		14.457	31.081
MOTA	925	N	$\operatorname{GLN}$	В	2	9.51		15.542	28.523
MOTA	926	H	GLN	В	2	9.75		16.474	28.251
MOTA	927	CA	GLN	В	2	8.18		15.058	28.242
MOTA	928	С	GLN	В	2	8.06	6	15.151	26.749
ATOM	929	0	GLN	В	2	8.52	23	16.140	26.133
ATOM	930	CB	GLN	В	2	7.15	55	15.976	28.856
ATOM	931	CG		В	2	5.73	9	15.732	28.373
ATOM	932	CD		В	2	4.74	4	16.365	29.284
ATOM	933	OE1	GLN		2	4.62	28	15.962	30.431
ATOM	934	NE2	GLN	В	2	4.02	24	17.367	28.784
ATOM	935	1HE2	GLN		2	3.34		17.830	29.349
ATOM	936	2HE2	GLN		2	4.16		17.665	27.839
ATOM	937	N		В	3	7.49		14.176	26.036
ATOM	938	Н		В	3	7.10		13.386	26.504
ATOM	939	CA		В	3	7.43		14.216	24.601
ATOM	940	C		В	3	5.95		14.097	24.184
ATOM	941	0		В	3	5.15		13.290	24.710
ATOM	942	CB		В	3	8.29		13.058	24.029
		CG1		В	3	9.74		13.232	24.534
ATOM	943			В	3	8.26		12.985	22.496
ATOM	944	CG2			3	10.62		12.068	24.143
ATOM	945	CD1		В	4	5.46		15.108	23.453
ATOM	946	N		В		6.04		15.108	23.226
ATOM	947	H		В	4			15.115	22.976
ATOM	948	CA		В	4	4.10		14.193	22.976
ATOM	949	C		В	4	4.03			
ATOM	950	0	THR	В	4	5.06	ЭÞ	13.755	21.203





# Figure 11R

ATOM	951	CB	THR B	4	3.616	16.548	22.647
ATOM	952	OG1	THR B	4	4.450	17.157	21.645
ATOM	953	HG1	THR B	4	4.123	18.080	21.442
ATOM	954	CG2	THR B	4	3.644	17.454	23.876
ATOM	955	N	LEU B	5	2.872	13.781	21.324
	956	H	LEU B	5	2.033	14.151	21.723
MOTA				5	2.837	12.795	20.265
ATOM	957	CA		5	2.183	13.415	19.047
MOTA	958	C	LEU B		1.677	12.720	18.142
MOTA	959	0	LEU B	5		11.577	20.762
ATOM	960	CB	LEU B	5	2.093		
MOTA	961	CG	LEU B	5	2.819	10.856	21.892
MOTA	962	CD1	LEU B	5	1.889	9.885	22.602
ATOM	963	CD2	LEU B	5	4.108	10.159	21.416
ATOM	964	N	TRP B	6	2.209	14.742	18.880
ATOM	965	H	TRP B	6	2.601	15.323	19.593
ATOM	966	CA	TRP B	6	1.683	15.364	17.690
ATOM	967	С	TRP B	6	2.581	14.978	16.509
ATOM	968	0	TRP B	6	2.159	14.851	15.349
ATOM	969	CB	TRP B	6	1.587	16.879	17.833
ATOM	970	CG	TRP B	6	0.652	17.339	18.921
ATOM	971	CD1	TRP B	6	0.955	17.584	20.232
ATOM	972	CD2	TRP B		-0.750	17.612	18.783
ATOM	973	NE1	TRP B	6	-0.167	17.989	20.913
ATOM	974	HE1	TRP B		-0.217	18.230	21.882
	975	CE2	TRP B		-1.224	18.013	20.048
ATOM		CE2	TRP B		-1.637	17.550	17.709
ATOM	976				-2.544	18.352	20.266
ATOM	977	CZ2			-2.947	17.885	17.921
ATOM	978	CZ3	TRP B		-3.394	18.281	19.185
ATOM	979	CH2	TRP B			14.809	16.738
MOTA	980	N	GLN B		3.896	14.809	17.650
MOTA	981	H	GLN B		4.267		15.689
MOTA	982	CA	GLN B		4.794	14.376	
ATOM	983	С	GLN E		5.361	13.043	16.096
MOTA	984	0	GLN E		5.221	12.586	17.243
ATOM	985	CB	GLN E		5.880	15.430	15.505
ATOM	986	CG	GLN E		5.353	16.704	14.804
ATOM	987	CD	GLN E		6.197	17.912	15.137
ATOM	988	OE1	GLN E		7.400	17.802	15.404
MOTA	989	NE2	GLN E	3 7	5.553	19.083	15.121
MOTA	990	1HE2	GLN E	3 7	6.040	19.931	15.330
MOTA	991	2HE2	GLN E	3 7	4.579	19.121	14.900
MOTA	992	N	ARG E	8	5.979	12.274	15.189
ATOM	993	H	ARG E	8	6.073	12.597	14.247
MOTA	994	CA	ARG E		6.505	10.985	15.573
MOTA	995	C	ARG E		7.577	11.198	16.610
ATOM	996	Ö	ARG E		8.395	12.130	16.515
MOTA	997	CB	ARG E		7.092	10.238	14.384
	998	CG	ARG E		6.132	10.018	13.237
ATOM ATOM	999	CD	ARG E		6.802	9.402	12.046
	1000	NE	ARG I		5.846	9.005	11.023
ATOM					4.872	9.080	11.237
ATOM	1001	HE	ARG I		6.217	8.552	9.828
ATOM	1002	CZ	ARG I		7.496	8.442	9.486
ATOM	1003	NH1				8.703	10.134
ATOM	1004	2HH1			8.211	8.098	8.580
ATOM	1005	1HH1			7.744	8.202	8.952
ATOM	1006	NH2	ARG I	3 8	5.279	0.202	0.752





# Figure $11\S$

ATOM	1007	1HH2	ARG B	8	5.540	7.860	8.050
ATOM	1008	2HH2	ARG B	8	4.312	8.281	9.196
MOTA	1009	N	PRO B	9	7.663	10.381	17.682
ATOM	1010	CA	PRO B	9	8.666	10.587	18.746
MOTA	1011	С	PRO B	9	10.065	10.196	18.315
MOTA	1012	0	PRO B	9	10.678	9.215	18.778
ATOM	1013	СВ	PRO B	9	8.148	9.682	19.878
ATOM	1013	CG	PRO B	9	7.315	8.607	19.206
	1015	CD	PRO B	9	6.708	9.323	18.004
ATOM			LEU B	10	10.685	10.969	17.400
ATOM	1016	N			10.303	11.746	16.998
MOTA	1017	H	LEU B	10			16.978
MOTA	1018	CA	LEU B	10	12.040	10.706	
MOTA	1019	C	LEU B	10	12.976	11.498	17.850
MOTA	1020	0	LEU B	10	12.880	12.733	18.018
MOTA	1021	CB	LEU B	10	12.250	11.170	15.554
MOTA	1022	CG	LEU B	10	11.427	10.386	14.551
ATOM	1023	CD1	LEU B	10	11.385	11.175	13.276
MOTA	1024	CD2	LEU B	10	11.956	8.947	14.355
MOTA	1025	N	VAL B	11	14.030	10.843	18.384
MOTA	1026	H	VAL B	11	14.148	9.866	18.206
ATOM	1027	CA	VAL B	11	15.018	11.517	19.223
ATOM	1028	C	VAL B	11	16.400	11.111	18.740
ATOM	1029	Ö	VAL B	11	16.581	10.201	17.911
ATOM	1030	CB	VAL B	11	14.857	11.100	20.699
ATOM	1031	CG1	VAL B	11	13.514	11.586	21.293
ATOM	1031	CG2	VAL B	11	15.038	9.573	20.903
	1032	N	THR B	12	17.485	11.739	19.232
MOTA			THR B	12	17.370	12.507	19.862
ATOM	1034	H				11.325	18.868
ATOM	1035	CA	THR B	12	18.843	10.284	19.837
MOTA	1036	C	THR B	12	19.377		21.082
MOTA	1037	0	THR B	12	19.237	10.352	
MOTA	1038	CB	THR B	12	19.830	12.520	18.820
MOTA	1039	OG1	THR B	12	19.389	13.483	17.876
MOTA	1040	HG1	THR B	12	20.028	14.252	17.848
MOTA	1041	CG2	THR B	12	21.234	12.075	18.399
ATOM	1042	N	ILE B	13	20.044	9.234	19.338
ATOM	1043	H	ILE B	13	20.135	9.130	18.348
ATOM	1044	CA	ILE B	13	20.641	8.239	20.176
MOTA	1045	С	ILE B	13	22.119	8.226	19.855
ATOM	1046	0	ILE B	13	22.579	8.817	18.865
ATOM	1047	CB	ILE B	13	19.993	6.870	19.879
MOTA	1048	CG1	ILE B	13	20.192	6.464	18.415
ATOM	1049	CG2	ILE B	13	18.482	6.893	20.206
ATOM	1050	CD1	ILE B	13	19.829	5.035	18.106
ATOM	1051	N	LYS B	14	22.973	7.618	20.661
ATOM	1052	H	LYS B	14	22.652	7.243	21.531
	1052	CA	LYS B	14	24.364	7.480	20.317
ATOM					24.680	6.029	20.477
ATOM	1054	C	LYS B	14		5.353	21.484
ATOM	1055	O	LYS B	14	24.353		
ATOM	1056	CB	LYS B	14	25.266	8.263	21.242
ATOM	1057	CG	LYS B	14	24.947	9.729	21.236
ATOM	1058	CD	LYS B	14	25.664	10.498	22.339
ATOM	1059	CE	LYS B	14	26.758	11.441	21.807
ATOM	1060	NZ	LYS B	14	28.026	10.781	21.440
ATOM	1061		LYS B	14	28.674	11.466	21.107
ATOM	1062	3HZ	LYS B	14	27.855	10.107	20.722





## Figure 11T

ATOM	1063	2HZ	LYS B	14	28	3.408	10.323	22.243
ATOM	1064	N	ILE B	15	25	5.214	5.390	19.425
ATOM	1065	H	ILE B	15	25	5.434	5.901	18.594
ATOM	1066	CA	ILE B	15	25	5.489	3.989	19.434
ATOM	1067	C	ILE B	15		5.832	3.981	18.750
ATOM	1068	Õ	ILE B	15		7.104	4.869	17.933
	1069	CB	ILE B	15		1.435	3.220	18.606
ATOM		CG1	ILE B	15		1.893	1.824	18.347
ATOM	1070			15		1.048	3.977	17.309
ATOM	1071	CG2	ILE B			3.830	0.996	17.645
ATOM	1072	CD1	ILE B	15			3.212	19.202
ATOM	1073	N	GLY B	16		7.812		19.202
MOTA	1074	H	GLY B	16		7.623	2.535	
ATOM	1075	CA	GLY B	16		9.175	3.336	18.677
MOTA	1076	С	GLY B	16		9.771	4.754	18.619
MOTA	1077	0	GLY B	16		0.737	4.970	17.902
ATOM	1078	N	GLY B	17		9.273	5.791	19.335
ATOM	1079	H	GLY B	17		3.453	5.660	19.892
ATOM	1080	CA	GLY B	17		9.924	7.105	19.302
MOTA	1081	С	GLY B	17	29	9.468	8.043	18.176
ATOM	1082	0	GLY B	17	29	9.984	9.155	17.933
ATOM	1083	N	GLN B	18	28	3.433	7.621	17.411
ATOM	1084	H	GLN B	18	28	3.046	6.711	17.560
ATOM	1085	CA	GLN B	18	2	7.834	8.449	16.348
ATOM	1086	С	GLN B	18	26	6.407	8.755	16.736
ATOM	1087	0	GLN B	18	25	5.678	7.953	17.353
MOTA	1088	CB	GLN B	18	2	7.810	7.645	15.045
MOTA	1089	CG	GLN B	18	2	7.247	6.204	15.146
ATOM	1090	CD	GLN B	18	2	7.572	5.333	13.924
ATOM	1091	OE1	GLN B	18	20	6.771	4.501	13.464
ATOM	1092	NE2	GLN B	18	28	8.766	5.531	13.393
ATOM	1093	1HE2	GLN B	18	2	9.057	5.005	12.594
ATOM	1094	2HE2	GLN B	18	2	9.388	6.209	13.786
ATOM	1095	N	LEU B	19	2	5.873	9.933	16.337
ATOM	1096	Н	LEU B	19	2	6.446	10.602	15.863
ATOM	1097	CA	LEU B	19	2	4.467	10.267	16.578
ATOM	1098	C	LEU B	19	2	3.633	9.622	15.490
ATOM	1099	Ō	LEU B	19		3.912	9.707	14.284
ATOM	1100	СB	LEU B	19		4.207	11.777	16.457
ATOM	1101	CG	LEU B	19		4.857	12.756	17.454
ATOM	1102	CD1	LEU B	19		4.739	12.335	18.880
ATOM	1103	CD2	LEU B	19		6.299	13.072	17.130
ATOM	1104	N	LYS B	20		2.450	9.085	15.850
ATOM	1105	H	LYS B	20		2.242	8.948	16.819
ATOM	1105	CA	LYS B	20		1.472	8.702	14.867
ATOM	1107	C	LYS B	20		0.121	9.105	15.417
ATOM	1107	0	LYS B	20		9.957	9.572	16.569
		CB	LYS B	20		1.496	7.200	14.560
MOTA	1109			20		2.904	6.653	14.507
MOTA	1110	CG		20		3.052	5.366	13.677
MOTA	1111	CD		20		3.052	5.603	12.145
ATOM	1112	CE	LYS B			3.893	6.758	11.699
ATOM	1113	NZ	LYS B	20		3.847	6.836	10.703
ATOM	1114	1HZ	LYS B	20			6.617	11.978
MOTA	1115		LYS B	20		4.843	7.597	12.116
ATOM	1116		LYS B	20		3.544	9.022	14.591
ATOM	1117		GLU B	21 21		9.068 9.200	8.712	13.650
ATOM	1118	Н	GLU B	Z 1	1	J. Z U U	0./12	10.00





# Figure 11U

ATOM	1119	CA	GLU B	21	17.735	9.366	15.008
ATOM	1120	C	GLU B	21	16.937	8.095	15.119
MOTA	1121	Ö	GLU B	21	17.117	7.103	14.376
ATOM	1122	CB	GLU B	21	17.143	10.314	13.983
		CG	GLU B	21	15.714	10.706	14.162
ATOM	1123				15.304	11.607	13.036
MOTA	1124	CD	GLU B	21			11.957
MOTA	1125	OE1	GLU B	21	14.971	11.051	
MOTA	1126	OE2	GLU B	21	15.338	12.854	13.174
MOTA	1127	N	ALA B	22	16.025	7.999	16.072
MOTA	1128	H	ALA B	22	15.825	8.792	16.648
MOTA	1129	CA	ALA B	22	15.300	6.783	16.315
ATOM	1130	С	ALA B	22	13.981	7.132	16.952
MOTA	1131	0	ALA B	22	13.756	8.153	17.632
ATOM	1132	CB	ALA B	22	16.095	5.865	17.235
ATOM	1133	N	LEU B	23	12.994	6.230	16.743
ATOM	1134	H	LEU B	23	13.195	5.379	16.257
MOTA	1135	CA	LEU B	23	11.639	6.408	17.180
ATOM	1136	C	LEU B	23	11.476	5.740	18.534
	1137	0	LEU B	23	11.814	4.564	18.746
MOTA			LEU B	23	10.775	5.665	16.192
ATOM	1138	CB		23	9.267	5.810	16.237
MOTA	1139	CG	LEU B			7.142	15.664
MOTA	1140	CD1	LEU B	23	8.807		
ATOM	1141	CD2	LEU B	23	8.648	4.625	15.482
MOTA	1142	N	LEU B	24	10.948	6.455	19.553
ATOM	1143	H	LEU B	24	10.775	7.433	19.435
ATOM	1144	CA	LEU B	24	10.613	5.838	20.849
MOTA	1145	С	LEU B	24	9.271	5.160	20.687
MOTA	1146	0	LEU B	24	8.208	5.764	20.418
ATOM	1147	CB	LEU B	24	10.564	6.878	21.971
ATOM	1148	CG	LEU B	24	11.828	7.750	22.075
ATOM	1149	CD1	LEU B	24	11.580	8.859	23.077
ATOM	1150	CD2	LEU B	24	13.099	6.955	22.388
ATOM	1151	N	ASP B	25	9.246	3.822	20.809
ATOM	1151	H	ASP B	25	10.025	3.347	21.218
		CA	ASP B	25	8.122	3.030	20.366
ATOM	1153			25	7.637	2.136	21.484
MOTA	1154	C			8.189	1.048	21.759
ATOM	1155	O	ASP B	25	8.613	2.196	19.189
ATOM	1156	CB	ASP B	25			18.511
MOTA	1157	CG	ASP B	25	7.528	1.421	
ATOM	1158	OD1		25	6.422	1.339	19.058
ATOM	1159	OD2	ASP B	25	7.800	0.897	17.426
ATOM	1160	N	THR B	26	6.547	2.465	22.157
ATOM	1161	H	THR B	26	6.067	3.314	21.938
ATOM	1162	CA	THR B	26	6.025	1.621	23.212
ATOM	1163	С	THR B	26	5.347	0.369	22.694
ATOM	1164	0	THR B	26	4.976	-0.550	23.451
ATOM	1165	CB	THR B	26	5.027	2.389	24.046
ATOM	1166	OG1	THR B	26	3.927	2.853	23.239
ATOM	1167	HG1	THR B	26	3.277	3.359	23.806
ATOM	1168	CG2	THR B	26	5.703	3.603	24.650
ATOM	1169	N N	GLY B	27	5.090	0.245	21.382
		H	GLY B	27	5.341	0.983	20.756
ATOM	1170		GLY B	27	4.457	-0.938	20.867
ATOM	1171	CA		27	5.475	-1.992	20.458
ATOM	1172	C	GLY B		5.121	-3.108	20.456
ATOM	1173	O	GLY B	27	6.792	-1.717	20.033
ATOM	1174	N	ALA B	28	0./32	- 1. / 1 /	40.493





# Figure 11 $\forall$

MOTA	1175	Н	ALA B	28	7.104	-0.832	20.841
ATOM	1176	CA	ALA B	28	7.800	-2.690	20.037
ATOM	1177	C	ALA B	28	8.371	-3.444	21.259
ATOM	1178	Õ	ALA B	28	8.840	-2.807	22.213
ATOM	1179	СВ	ALA B	28	8.924	-1.936	19.358
	1180	N	ASP B	29	8.459	-4.787	21.289
ATOM					8.082	-5.325	20.535
MOTA	1181	H	ASP B	29			
MOTA	1182	CA	ASP B	29	9.121	-5.441	22.452
ATOM	1183	С	ASP B	29	10.608	-5.219	22.404
MOTA	1184	0	ASP B	29	11.345	-5.264	23.412
MOTA	1185	CB	ASP B	29	8.965	-6.975	22.447
ATOM	1186	CG	ASP B	29	7.551	-7.477	22.774
MOTA	1187	OD1	ASP B	29	6.683	-6.693	23.169
MOTA	1188	OD2	ASP B	29	7.350	-8.686	22.616
ATOM	1189	N	ASP B	30	11.164	-5.157	21.171
ATOM	1190	Н	ASP B	30	10.577	-5.063	20.367
ATOM	1191	CA	ASP B	30	12.609	-5.217	20.880
ATOM	1192	C	ASP B	30	13.048	-3.886	20.335
ATOM	1193	Ö	ASP B	30	12.269	-3.055	19.817
ATOM	1194	CB	ASP B	30	12.833	-6.226	19.735
ATOM	1195	CG	ASP B	30	12.477	-7.675	20.099
		OD1	ASP B	30	13.197	-8.272	20.908
ATOM	1196			30	11.494	-8.237	19.569
ATOM	1197	OD2	ASP B		14.387	-3.692	20.227
ATOM	1198	Ŋ	THR B	31			20.586
ATOM	1199	H	THR B	31	15.018	-4.380	
ATOM	1200	CA	THR B		14.981	-2.530	19.614
ATOM	1201	C	THR B		15.578	-2.979	18.260
ATOM	1202	0	THR B		16.246	-4.020	18.123
ATOM	1203	CB	THR B		16.036	-2.004	20.557
ATOM	1204	OG1	THR B		15.378	-1.376	21.645
MOTA	1205	HG1	THR B		16.052	-1.016	22.290
MOTA	1206	CG2	THR B		16.944	-0.960	19.904
MOTA	1207	N	VAL B		15.237	-2.283	17.150
MOTA	1208	H	VAL B		14.703	-1.442	17.237
MOTA	1209	CA	VAL B		15.626	-2.722	15.806
MOTA	1210	С	VAL B		16.303	-1.566	15.132
ATOM	1211	0	VAL B	32	15.779	-0.428	14.995
ATOM	1212	CB	VAL B	32	14.407	-3.126	14.964
ATOM	1213	CG1	VAL B	32	14.820	-3.703	13.596
ATOM	1214	CG2	VAL B	32	13.556	-4.102	15.703
ATOM	1215	N	LEU B	33	17.563	-1.756	14.720
ATOM	1216	H	LEU B	33	17.984	-2.658	14.814
MOTA	1217	CA	LEU B		18.347	-0.697	14.138
ATOM	1218	C	LEU B		18.610	-1.009	12.685
ATOM	1219	0	LEU B		18.685	-2.162	12.205
ATOM	1220	CB	LEU B		19.679	-0.628	14.856
ATOM	1221	ĊĠ	LEU B		19.698	0.363	16.031
MOTA	1222	CD1	LEU B		18.425	0.321	16.891
MOTA	1223	CD2	LEU B		20.929	0.179	16.889
ATOM	1224	N N	GLU B		18.786	0.078	11.899
ATOM	1225	Н	GLU B		18.619	0.991	12.271
ATOM	1225	CA	GLU B		19.218	0.041	10.488
ATOM	1227	CA	GLU B		20.478	-0.774	10.399
	1227	0	GLU B		21.374	-0.835	11.272
ATOM		CB	GLU B		19.536	1.460	9.996
ATOM	1229				20.722	2.088	10.761
MOTA	1230	CG	GLU B	34	20.722	2.000	10.761





# Figure 11W

			~	~ 4	01 005	2 512	10 214
MOTA	1231	$^{\mathrm{CD}}$	GLU B	34	21.085	3.512	10.314
MOTA	1232	OE1	GLU B	34	20.285	4.466	10.500
ATOM	1233	OE2	GLU B	34	22.211	3.703	9.775
MOTA	1234	N	GLU B	35	20.673	-1.367	9.205
MOTA	1235	H	GLU B	35	20.011	-1.227	8.468
MOTA	1236	CA	GLU B	35	21.802	-2.205	8.930
ATOM	1237	C	GLU B	35	23.096	-1.520	9.321
ATOM	1238	Ö	GLU B	35	23.391	-0.379	8.916
ATOM	1239	CB	GLU B	35	21.741	-2.479	7.439
ATOM	1240	CG	GLU B	35	22.795	-3.380	6.883
		CD	GLU B	35	22.987	-4.587	7.744
ATOM	1241			35	21.980	-5.258	8.118
ATOM	1242	OE1	GLU B			-4.860	8.048
MOTA	1243	OE2	GLU B	35	24.149		10.157
MOTA	1244	N	MET B	36	23.926	-2.106	
ATOM	1245	H	MET B	36	23.654	-2.953	10.613
MOTA	1246	CA	MET B	36	25.232	-1.559	10.441
MOTA	1247	С	MET B	36	26.146	-2.687	10.815
ATOM	1248	0	MET B	36	25.731	-3.783	11.257
ATOM	1249	CB	MET B	36	25.251	-0.424	11.497
ATOM	1250	CG	MET B	36	24.626	-0.724	12.881
ATOM	1251	SD	MET B	36	24.722	0.719	13.988
ATOM	1252	CE	MET B	36	23.132	1.586	13.692
MOTA	1253	N	SER B	37	27.441	-2.551	10.593
ATOM	1254	H	SER B	37	27.783	-1.726	10.144
ATOM	1255	CA	SER B	37	28.321	-3.608	11.011
ATOM	1256	С	SER B	37	28.721	-3.352	12.442
ATOM	1257	Ō	SER B	37	29.402	-2.369	12.788
ATOM	1258	СВ	SER B	37	29.567	-3.622	10.109
ATOM	1259	OG	SER B	37	29.231	-3.908	8.750
ATOM	1260	HG	SER B	37	30.057	-3.911	8.187
ATOM	1261	N	LEU B	38	28.469	-4.295	13.366
ATOM	1262	H	LEU B	38	27.948	-5.123	13.117
ATOM	1263	CA	LEU B	38	29.073	-4.232	14.714
ATOM	1264	C	LEU B	38	30.132	-5.342	14.895
ATOM	1265	Ö	LEU B	38	30.070	-6.357	14.197
ATOM	1266	СВ	LEU B	38	27.986	-4.237	15.802
ATOM	1267	CG	LEU B	38	27.005	-3.039	15.750
ATOM	1268	CD1	LEU B	38	25.885	-3.214	16.788
ATOM	1269	CD2	LEU B	38	27.707	-1.696	16.017
ATOM	1270	N	PRO B	39	31.119	-5.160	15.804
ATOM	1271	CA	PRO B	39	32.199	-6.116	16.052
ATOM	1271	C	PRO B	39	31.767	-7.223	17.028
ATOM	1272	0	PRO B	39	31.448	-6.942	18.185
		CB	PRO B	39	33.347	-5.276	16.625
ATOM	1274			39	32.634	-4.148	17.370
ATOM	1275	CG	PRO B		31.385	-3.916	16.523
ATOM	1276	CD	PRO B	39	31.770	-8.481	16.559
ATOM	1277	N	GLY B	40	32.036	-8.641	15.598
ATOM	1278	H	GLY B	40			
ATOM	1279	CA	GLY B	40	31.420	-9.658	17.353
ATOM	1280	C	GLY B	40	30.679	-10.723	16.539
ATOM	1281	0	GLY B		30.647	-10.671	15.308
ATOM	1282	N	LYS B		30.098	-11.699	17.255
ATOM	1283	H	LYS B		30.164	-11.656	18.261
ATOM	1284	CA	LYS B		29.399	-12.861	16.702
ATOM	1285	C	LYS B		27.971	-12.923	17.245
MOTA	1286	0	LYS B	41	27.743	-12.700	18.436





# Figure 11X

MOTA	1287	CB	LYS B	41	30.154 -14.152 17.048
ATOM	1288	CG	LYS B	41	31.537 -14.221 16.384
ATOM	1289	$^{\rm CD}$	LYS B	41	32.192 -15.580 16.651
ATOM	1290	CE	LYS B	41	33.566 -15.642 15.983
ATOM	1291	NZ	LYS B	41	34.198 -16.956 16.183
ATOM	1292	1HZ	LYS B	41	35.102 -16.968 15.732
ATOM	1293	3HZ	LYS B	41	33.612 -17.674 15.782
ATOM	1294	2HZ	LYS B	41	34.312 -17.128 17.172
ATOM	1295	N	TRP B	42	27.018 -13.228 16.351
	1296	H	TRP B	42	27.307 -13.458 15.411
MOTA		CA	TRP B	42	25.597 -12.929 16.521
ATOM	1297			42	24.723 -14.179 16.405
ATOM	1298	C			
ATOM	1299	0	TRP B	42	
MOTA	1300	CB	TRP B	42	
MOTA	1301	CG	TRP B	42	26.127 -10.687 15.390
MOTA	1302	CD1	TRP B	42	26.651 -10.197 14.244
MOTA	1303	CD2	TRP B	42	26.739 -9.913 16.467
MOTA	1304	NE1	TRP B	42	27.548 -9.191 14.533
MOTA	1305	HE1	TRP B	42	28.067 -8.702 13.818
ATOM	1306	CE2	TRP B	42	27.664 -8.995 15.893
ATOM	1307	CE3	TRP B	42	26.640 -9.923 17.875
ATOM	1308	CZ2	TRP B	42	28.443 -8.136 16.680
ATOM	1309	CZ3	TRP B	42	27.426 -9.075 18.673
ATOM	1310	CH2	TRP B	42	28.318 -8.171 18.077
ATOM	1311	N	LYS B	43	23.416 -13.980 16.617
ATOM	1312	Н	LYS B	43	23.105 -13.044 16.840
ATOM	1313	CA	LYS B	43	22.378 -14.995 16.526
ATOM	1314	C	LYS B	43	21.368 -14.507 15.478
ATOM	1315	Õ	LYS B	43	20.743 -13.472 15.706
ATOM	1316	СВ	LYS B	43	21.694 -15.196 17.893
ATOM	1317	CG	LYS B	43	22.641 -15.623 19.034
ATOM	1318	CD	LYS B	43	22.409 -14.814 20.323
ATOM	1319	CE	LYS B	43	22.767 -13.327 20.182
ATOM	1320	NZ	LYS B	43	24.214 -13.113 20.015
ATOM	1321	1HZ	LYS B	43	24.400 -12.125 19.924
ATOM	1322	3HZ	LYS B	43	24.532 -13.593 19.185
ATOM	1323	2HZ	LYS B	43	24.702 -13.476 20.821
	1324	N	PRO B	44	21.175 -15.204 14.341
MOTA	1325	CA	PRO B	44	20.139 -14.835 13.382
MOTA				44	18.765 -14.997 14.044
ATOM	1326	C	PRO B		18.573 -15.902 14.860
MOTA	1327	O	PRO B	44	20.341 -15.761 12.180
ATOM	1328	CB	PRO B	44	
ATOM	1329	CG	PRO B	44	
ATOM	1330	CD	PRO B	44	21.837 -16.434 13.933
ATOM	1331	N	LYS B	45	17.825 -14.101 13.712
MOTA	1332	H	LYS B	45	17.994 -13.483 12.944
ATOM	1333	CA	LYS B	45	16.523 -14.088 14.339
ATOM	1334	C	LYS B	45	15.519 -13.590 13.329
MOTA	1335	0	LYS B	45	15.829 -12.838 12.379
MOTA	1336	CB	LYS B	45	16.558 -13.149 15.560
MOTA	1337	CG	LYS B	45	15.469 -13.442 16.579
MOTA	1338	CD	LYS B	45	15.256 -12.254 17.501
ATOM	1339	CE	LYS B	45	14.131 -12.461 18.469
MOTA	1340	NZ	LYS B	45	14.549 -13.442 19.474
ATOM	1341	1HZ	LYS B	45	13.805 -13.588 20.126
ATOM	1342		LYS B	45	15.355 -13.101 19.958





# Figure 11 Y

MOTA	1343	2HZ	LYS E	3 45	14.772 -14.306 19.023
ATOM	1344	N	MET E	3 46	14.240 -14.005 13.416
MOTA	1345	H	MET E	3 46	13.991 -14.705 14.085
ATOM	1346	CA	MET E	3 46	13.203 -13.472 12.570
ATOM	1347	C	MET E	3 46	12.291 -12.623 13.425
ATOM	1348	Ō	MET E		11.782 -13.063 14.471
ATOM	1349	CB	MET E		12.383 -14.616 12.016
ATOM	1350	CG	MET E		13.153 -15.586 11.187
ATOM	1351	SD	MET E		12.977 -15.188 9.473
ATOM	1351	CE	MET E		13.566 -16.690 8.775
		N	ILE E		11.933 -11.379 13.030
MOTA	1353		ILE E		12.327 -10.991 12.196
ATOM	1354	H			10.971 -10.568 13.797
ATOM	1355	CA			9.761 -10.233 12.962
ATOM	1356	C	ILE E		
MOTA	1357	0	ILE E		
MOTA	1358	CB	ILE E		11.608 -9.294 14.385
MOTA	1359	CG1	ILE E		12.345 -8.459 13.318
ATOM	1360	CG2	ILE E		12.542 -9.638 15.494
MOTA	1361	CD1	ILE E		12.789 -7.123 13.851
MOTA	1362	N	GLY E		8.557 -10.136 13.558
MOTA	1363	H	GLY E		8.484 -10.249 14.549
MOTA	1364	CA	GLY E		7.365 -9.872 12.800
ATOM	1365	С	GLY E	3 48	6.826 -8.512 13.141
ATOM	1366	0	GLY E	3 48	7.136 -7.832 14.149
ATOM	1367	N	GLY E	3 49	5.940 -8.027 12.306
MOTA	1368	H	GLY F	3 49	5.668 -8.562 11.506
ATOM	1369	CA	GLY E	3 49	5.336 -6.745 12.493
ATOM	1370	С	GLY E	3 49	4.082 -6.786 11.674
ATOM	1371	0	GLY E	3 49	3.561 -7.847 11.273
ATOM	1372	N	ILE E		3.531 -5.634 11.315
ATOM	1373	H	ILE E		4.015 -4.777 11.492
ATOM	1374	CA	ILE E		2.247 -5.573 10.673
ATOM	1375	C	ILE E		2.118 -6.456 9.420
ATOM	1376	Õ	ILE E		1.175 -7.253 9.215
ATOM	1377	CB	ILE E		1.982 -4.071 10.391
ATOM	1378	CG1	ILE E		1.005 -3.539 11.396
ATOM	1379	CG2	ILE E		1.610 -3.739 8.922
ATOM	1380	CD1	ILE I		-0.391 -4.077 11.252
ATOM	1381			3 51	3.113 -6.410 8.519
					3.957 -5.920 8.737
ATOM	1382	H	GLY I	3 51	2.926 -7.075 7.259
ATOM	1383	CA			3.671 -8.391 7.077
ATOM	1384	C			
ATOM	1385	0		3 51	
ATOM	1386	N		B 52	4.296 -8.982 8.116
MOTA	1387	H		B 52	4.227 -8.580 9.029
MOTA	1388	CA	GLY I		5.053 -10.190 7.874
ATOM	1389	C	GLY I		6.334 -10.178 8.678
MOTA	1390	0	GLY I		6.519 -9.421 9.657
MOTA	1391	N	PHE I		7.325 -11.015 8.343
MOTA	1392	H		B 53	7.227 -11.603 7.540
MOTA	1393	CA		B 53	8.542 -11.096 9.110
MOTA	1394	C		B 53	9.727 -10.584 8.315
MOTA	1395	0	PHE I	B 53	9.780 -10.618 7.075
MOTA	1396	CB	PHE I	B 53	8.804 -12.555 9.542
MOTA	1397	CG	PHE 1	B 53	7.850 -13.023 10.592
MOTA	1398	CD1	PHE 1	B 53	6.513 -13.277 10.279





# Figure 11Z

MOTA	1399	CD2	PHE I	B 53	3	-	-13.192	11.918
ATOM	1400	CE1	PHE I	B 53	3	5.620	-13.697	11.253
ATOM	1401	CE2	PHE I	B 53	3	7.382	-13.615	12.903
ATOM	1402	CZ	PHE I	B 53	3	6.052	-13.868	12.574
ATOM	1403	N	ILE I	B 54	1	10.758	-10.126	8.985
ATOM	1404	Н		B 54	1	10.665	-9.922	9.960
ATOM	1405	CA		B 54		12.029	-9.910	8.338
ATOM	1406	C		B 54		13.089	-10.648	9.134
ATOM	1407	Õ		B 54		12.952	-11.006	10.325
ATOM	1407	CB		B 54		12.390	-8.444	8.236
MOTA	1409	CG1		B 54		12.386	-7.775	9.611
ATOM	1410	CG2		B 54		11.460	-7.770	7.218
		CD1		B 54		13.113	-6.438	9.590
MOTA	1411			B 5!		14.272	-10.852	8.523
ATOM	1412	N				14.272	-10.599	7.562
ATOM	1413	H		B 5			-11.431	9.216
ATOM	1414	CA		B 5!		15.403		
MOTA	1415	C		B 5!		16.274	-10.324	9.732
MOTA	1416	0		B 5!		16.620	-9.328	9.047
MOTA	1417	CB		B 5!		16.222	-12.237	8.245
ATOM	1418	CG		B 5		15.638	-13.596	8.063
ATOM	1419	CD	LYS	B 5!		16.299	-14.348	6.953
ATOM	1420	CE	LYS	B 5!		15.311	-14.520	5.813
ATOM	1421	NZ	LYS	B 5!	5	15.757	-15.577	4.897
MOTA	1422	1HZ	LYS	B 5!	5	15.095	-15.676	4.154
MOTA	1423	3HZ	LYS	B 5	5	15.830	-16.441	5.395
ATOM	1424	2HZ		B 5!	5	16.650	-15.334	4.518
ATOM	1425	N		B 5		16.880	-10.547	10.910
ATOM	1426	H		B 5		16.741	-11.418	11.382
ATOM	1427	CA		B 5		17.732	-9.578	11.534
ATOM	1428	C		B 5		18.884	-10.304	12.184
ATOM	1429	Ö		B 5		18.884	-11.539	12.367
ATOM	1430	CB		B 5		16.912	-8.819	12.609
ATOM	1431	CG1		B 5		15.865	-7.943	11.921
ATOM	1432	CG2		B 5		16.215	-9.788	13.599
ATOM	1433	N		B 5		19.958	-9.593	12.591
ATOM	1434	H		B 5		20.030	-8.624	12.353
		CA		B 5		21.050	-10.193	13.386
ATOM	1435			в 5 В 5		20.963	-9.608	14.804
ATOM	1436	C		в 5 В 5		20.903	-8.395	15.053
ATOM	1437	O						12.817
ATOM	1438	CB	ARG			22.426	-9.873 -10.437	11.439
ATOM	1439	CG	ARG			22.664		
ATOM	1440	CD	ARG			24.012	-10.065	10.899
ATOM	1441	NE		B 5		24.280	-10.697	9.617
MOTA	1442	HE	ARG			23.592	-11.323	9.250
ATOM	1443	CZ	ARG			25.392	-10.478	8.921
ATOM	1444	NH1	ARG			26.337	-9.650	9.353
ATOM	1445	2HH1	ARG			26.223	-9.171	10.224
ATOM	1446	1HH1	ARG			27.163	-9.505	8.808
ATOM	1447	NH2	ARG			25.561	-11.104	7.760
ATOM	1448	1HH2	ARG	B 5	7	26.392	-10.950	7.225
MOTA	1449	2HH2	ARG	B 5	7	24.857	-11.729	7.422
ATOM	1450	N		B 5	8	20.997	-10.489	15.832
ATOM	1451	H	GLN			21.176	-11.456	15.650
ATOM	1452	CA	GLN			20.780	-10.072	17.206
ATOM	1453	C	GLN			22.108	-9.886	17.882
ATOM	1454	Ō	GLN			22.918	-10.815	18.038





### Figure 11aa

ATOM	1455	СВ	GLN E	3 58	20.051	-11.190	17.932
ATOM	1456	CG	GLN E		19.765	-10.845	19.366
ATOM	1457	CD	GLN E		19.179	-12.003	20.112
ATOM	1458	OE1	GLN E		19.712	-12.472	21.101
ATOM	1459	NE2	GLN E		18.055	-12.476	19.623
ATOM	1460	1HE2	GLN E		17.598		20.063
ATOM	1461	2HE2	GLN E			-13.249	
ATOM	1462	Znez N	TYR E		17.647	-12.066	18.807
ATOM	1462	H			22.416	-8.692	18.422
ATOM	1463	г СА	TYR E		21.788	-7.921	18.311
			TYR E		23.631	-8.486	19.161
ATOM	1465	C	TYR E		23.244	-8.290	20.607
ATOM	1466	O	TYR E		22.178	-7.728	20.927
ATOM	1467	CB	TYR E		24.387	-7.241	18.653
ATOM	1468	CG	TYR E		24.271	-7.075	17.149
ATOM	1469	CD1	TYR E		23.045	-7.242	16.494
ATOM	1470	CD2	TYR E		25.385	-6.753	16.374
ATOM	1471	CE1	TYR E		22.939	-7.093	15.112
ATOM	1472	CE2	TYR E		25.291	-6.603	14.995
MOTA	1473	CZ	TYR E		24.068	-6.774	14.365
ATOM	1474	OH	TYR E		24.018	-6.620	13.010
ATOM	1475	HH	TYR E		24.926	-6.394	12.658
ATOM	1476	N	ASP E		24.010	-8.785	21.596
ATOM	1477	H	ASP E		24.852	-9.276	21.372
ATOM	1478	CA	ASP E		23.644	-8.624	22.992
ATOM	1479	C	ASP E		24.556	-7.595	23.615
ATOM	1480	0	ASP E		25.654	-7.261	23.125
ATOM	1481	CB	ASP E		23.789	-9.920	23.777
ATOM	1482	CG	ASP E		22.803	-10.960	23.332
ATOM	1483	OD1	ASP E		21.619	-10.634	23.032
ATOM	1484	OD2	ASP E		23.208	-12.126	23.273
ATOM	1485	N	GLN E		24.156	-7.022	24.774
ATOM	1486	H	GLN E		23.252	-7.234	25.146
ATOM ATOM	1487	CA C	GLN E		25.011	-6.086	25.519
ATOM	1488		GLN E		25.411	-4.866	24.746
ATOM	1489 1490	O CB	GLN E		26.560	-4.382	24.832
ATOM	1491	CG			26.269	-6.763	26.028
ATOM	1491	CD	GLN E		26.020	-8.038	26.753
ATOM	1493	OE1	GLN E		25.714 24.572	-7.766 -7.455	28.185 28.548
ATOM	1494		GLN E		26.744	-7.433	29.014
ATOM	1495		GLN B		26.620	-7.675	29.992
ATOM	1496	2HE2	GLN B		27.654	-8.073	28.669
ATOM	1497	N	ILE B		24.539	-4.257	23.933
ATOM	1498	Н	ILE B		23.628	-4.648	23.801
ATOM	1499	CA	ILE B		24.878	-3.047	23.238
ATOM	1500	C	ILE B		24.571	-1.885	24.144
ATOM	1501	Ö	ILE B		23.515	-1.819	24.819
MOTA	1502	CB	ILE B		24.097	-2.922	21.912
MOTA	1503	CG1	ILE B		24.310	-4.170	21.094
ATOM	1504	CG2	ILE B		24.568	-1.709	21.054
ATOM	1505	CD1	ILE B		25.794	-4.479	20.878
ATOM	1506	N	LEU B		25.485	-0.912	24.304
ATOM	1507	Н	LEU B		26.403	-1.028	23.926
ATOM	1508	CA	LEU B		25.192	0.322	25.015
ATOM	1509	C	LEU B		24.630	1.296	24.030
ATOM	1510	Ō	LEU B		25.239	1.658	22.995
					- · - · ·		





## Figure 11bb

ATOM	1511	CB	LEU E	63	26.436	0.970	25.590
MOTA	1512	CG	LEU E	63	26.186	2.358	26.226
ATOM	1513	CD1	LEU E		25.486	2.261	27.576
ATOM	1514	CD2	LEU E		27.468	3.162	26.382
MOTA	1515	N	ILE E	64	23.492	1.946	24.358
MOTA	1516	H	ILE E	64	22.958	1.643	25.148
ATOM	1517	CA	ILE E	64	23.003	3.068	23.617
ATOM	1518	C	ILE E		22.872	4.194	24.612
							25.846
ATOM	1519	0			22.915	4.007	
MOTA	1520	CB	ILE E		21.634	2.701	22.989
ATOM	1521	CG1	ILE E	64	21.825	1.521	22.029
MOTA	1522	CG2	ILE E	64	20.982	3.894	22.246
MOTA	1523	CD1	ILE E	64	20.593	1.096	21.260
ATOM	1524	N	GLU E		22.803	5.460	24.172
	1525	H	GLU E		23.013	5.664	23.216
ATOM							
MOTA	1526	CA	GLU E		22.432	6.551	25.037
MOTA	1527	C	GLU E		21.242	7.194	24.373
MOTA	1528	0	GLU E	65	21.312	7.729	23.257
MOTA	1529	CB	GLU E	65	23.497	7.615	25.131
ATOM	1530	CG	GLU E		24.787	7.196	25.761
ATOM	1531	CD	GLU E		25.694	8.385	26.076
ATOM	1532	OE1	GLU E		25.170	9.510	26.311
MOTA	1533	OE2	GLU E	65	26.938	8.200	26.092
ATOM	1534	N	ILE E	66	20.078	7.240	25.035
MOTA	1535	Н	ILE E	66	20.010	6.835	25.947
ATOM	1536	CA	ILE E	66	18.907	7.865	24.462
ATOM	1537	C	ILE E		18.777	9.195	25.145
ATOM	1538	0	ILE E		18.591	9.303	26.379
ATOM	1539	CB	ILE E		17.713	6.995	24.790
MOTA	1540	CG1	ILE E		17.916	5.583	24.335
MOTA	1541	CG2	ILE E	66	16.405	7.544	24.177
ATOM	1542	CD1	ILE E	66	16.888	4.677	24.884
MOTA	1543	N	CYS E		18.965	10.325	24.437
ATOM	1544	H	CYS E		19.201	10.268	23.467
ATOM	1545	CA	CYS E		18.833	11.663	25.049
ATOM	1546	C	CYS E		19.637	11.781	26.319
MOTA	1547	0	CYS E		19.235	12.400	27.328
MOTA	1548	CB	CYS E	67	17.387	12.023	25.319
ATOM	1549	SG	CYS E	67	16.407	12.259	23.821
ATOM	1550	N	GLY E	68	20.830	11.180	26.383
ATOM	1551	H	GLY E		21.158	10.646	25.604
ATOM	1552	CA	GLY E		21.654	11.288	27.558
ATOM	1553	C	GLY E		21.464	10.185	28.584
MOTA	1554	0	GLY E		22.174	10.128	29.606
MOTA	1555	N	HIS E	69	20.513	9.255	28.425
ATOM	1556	H	HIS E	69	19.924	9.282	27.618
MOTA	1557	CA	HIS E		20.304	8.199	29.391
ATOM	1558	C	HIS E		20.861	6.936	28.811
ATOM	1559	0	HIS E		20.589	6.560	27.647
MOTA	1560	CB	HIS E		18.832	7.992	29.654
MOTA	1561	CG	HIS E	69	18.175	9.203	30.223
MOTA	1562	ND1	HIS E	69	17.504	9.195	31.435
MOTA	1563	HD1	HIS E	69	17.383	8.402	32.032
ATOM	1564	CD2	HIS E		18.122	10.470	29.729
ATOM	1565	CE1	HIS E		17.070	10.429	31.626
ATOM	1566	NE2	HIS E		17.410	11.240	30.635
AION	1000	1417	1110 E	0 9	17.410	11.240	30.033





### Figure $11_{\text{CC}}$

ATOM	1567	N	LYS B	70	21.751	6.217	29.499
ATOM	1568	Н	LYS B	70	22.025	6.512	30.414
ATOM	1569	CA	LYS B	70	22.326	5.020	28.945
ATOM	1570	C	LYS B	70	21.386	3.854	29.145
ATOM	1571	Ö	LYS B	70	20.627	3.725	30.120
ATOM	1572	СВ	LYS B	70	23.613	4.678	29.663
ATOM	1573	CG	LYS B	70	24.694	5.655	29.379
ATOM	1574	CD	LYS B	70	25.739	5.524	30.444
ATOM	1575	CE	LYS B	70	27.048	6.090	30.011
ATOM	1576	NZ	LYS B	70	26.948	7.548	30.000
ATOM	1577	1HZ	LYS B	70	27.821	7.940	29.711
				70	26.725		30.919
ATOM	1578	3HZ	LYS B		26.230	7.874	
MOTA	1579	2HZ	LYS B	70		7.828	29.363
ATOM	1580	N	ALA B	71	21.512	2.849	28.284
ATOM	1581	H	ALA B	71	22.141	2.934	27.512
ATOM	1582	CA	ALA B	71	20.762	1.630	28.432
ATOM	1583	C	ALA B	71	21.629	0.576	27.805
ATOM	1584	0	ALA B	71	22.463	0.830	26.912
ATOM	1585	CB	ALA B	71	19.452	1.726	27.737
MOTA	1586	N	ILE B	72	21.547	-0.681	28.237
MOTA	1587	H	ILE B	72	20.864	-0.925	28.926
MOTA	1588	CA	ILE B	72	22.424	-1.698	27.730
MOTA	1589	С	ILE B	72	21.615	-2.938	27.462
ATOM	1590	0	ILE B	72	20.909	-3.490	28.330
MOTA	1591	CB	ILE B	72	23.524	-1.999	28.737
ATOM	1592	CG1	ILE B	72	24.322	-0.735	29.090
ATOM	1593	CG2	ILE B	72	24.442	-3.037	28.153
ATOM	1594	CD1	ILE B	72	25.374	-1.012	30.163
ATOM	1595	N	GLY B	73	21.609	-3.446	26.235
ATOM	1596	Н	GLY B	73	22.204	-3.054	25.534
MOTA	1597	CA	GLY B	73	20.707	-4.545	26.062
ATOM	1598	C	GLY B	73	20.828	-5.084	24.663
ATOM	1599	Ō	GLY B	73	21.754	-4.831	23.863
ATOM	1600	N	THR B	74	19.856	-5.905	24.271
ATOM	1601	H	THR B	74	19.086	-6.088	24.882
ATOM	1602	CA	THR B	74	19.869	-6.548	22.988
ATOM	1603	C	THR B	74	19.363	-5.590	21.931
ATOM	1604	Ö	THR B	74	18.338	-4.870	22.053
ATOM	1605	CB	THR B	74	19.011	-7.801	23.074
ATOM	1605	OG1	THR B	74	19.611	-8.683	24.013
ATOM	1607	HG1	THR B	74	19.068	-9.519	24.013
ATOM	1607	CG2	THR B	74			
					18.817	-8.496	21.705
ATOM	1609	N	VAL B	75	20.028	-5.620	20.762
ATOM	1610	H	VAL B	75	20.835	-6.203	20.666
MOTA	1611	CA	VAL B	75	19.630	-4.837	19.611
ATOM	1612	C	VAL B	75	19.600	-5.771	18.426
ATOM	1613	0	VAL B	75	20.444	-6.673	18.230
ATOM	1614	CB	VAL B	75	20.667	-3.712	19.395
ATOM	1615	CG1	VAL B	75	20.473	-3.002	18.046
ATOM	1616	CG2	VAL B	75	20.679	-2.708	20.567
MOTA	1617	N	LEU B	76	18.557	-5.647	17.565
ATOM	1618	H	LEU B	76	17.822	-5.000	17.767
MOTA	1619	CA	LEU B	76	18.444	-6.427	16.324
ATOM	1620	С	LEU B	76	18.736	-5.487	15.144
MOTA	1621	0	LEU B	76	18.239	-4.343	15.040
MOTA	1622	CB	LEU B	76	17.028	-7.021	16.158





# Figure 11dd

ATOM	1623	CG	LEU B	76	16.	427	-7.612	17.449
ATOM	1624	CD1	LEU B	76	14.	992	-8.075	17.263
MOTA	1625	CD2	LEU B	76	17.	266	-8.758	18.019
ATOM	1626	N	VAL B	77		607	-5.900	14.222
		Н	VAL B	77		985	-6.824	14.276
ATOM	1627			77		027	-5.042	13.133
ATOM	1628	CA		77		570	-5.662	11.842
MOTA	1629	C	VAL B				-6.883	11.598
MOTA	1630	0	VAL B	77		678		13.191
MOTA	1631	CB	VAL B	77		563	-4.905	
MOTA	1632	CG1	VAL B	77		129	-4.202	11.944
MOTA	1633	CG2	VAL B	77		030	-4.166	14.470
ATOM	1634	N	GLY B	78		978	-4.915	10.943
ATOM	1635	H	GLY B	78		841	-3.941	11.121
MOTA	1636	CA	GLY B	78		523	-5.475	9.705
ATOM	1637	С	GLY B	78	18.	019	-4.338	8.874
ATOM	1638	0	GLY B	78	18.	130	-3.142	9.223
ATOM	1639	N	PRO B	79	17.	408	-4.596	7.722
ATOM	1640	CA	PRO B	79	16.	954	-3.535	6.834
MOTA	1641	С	PRO B	79	15.	635	-2.872	7.280
MOTA	1642	Ö	PRO B	79	14.	609	-2.877	6.565
ATOM	1643	CB	PRO B	79	16.	804	-4.274	5.492
ATOM	1644	CG	PRO B	79		463	-5.712	5.881
ATOM	1645	CD	PRO B	79		159	-5.959	7.189
ATOM	1646	N	THR B	80		574	-2.247	8.458
		H	THR B	80		374	-2.242	9.058
ATOM	1647	СA	THR B	80		.364	-1.583	8.865
ATOM	1648	CA	THR B	80		312	-0.189	8.228
ATOM	1649	0	THR B	80		.349	0.471	8.001
ATOM	1650	_	THR B	80		.250	-1.512	10.410
ATOM	1651	CB		80		.079	-0.802	10.806
ATOM	1652	OG1	THR B			.022	-0.766	11.804
ATOM	1653	HG1	THR B	80		.519	-0.901	11.062
MOTA	1654	CG2	THR B	80		.137	0.354	7.885
ATOM	1655	N	PRO B	81			1.747	7.379
ATOM	1656	CA	PRO B	81		.036		8.484
ATOM	1657	C	PRO B	81		.363	2.732	
ATOM	1658	0	PRO B	81		.791	3.880	8.250
MOTA	1659	CB	PRO B	81		.548	1.912	6.982
MOTA	1660	CG	PRO B	81		.819	0.674	7.488
MOTA	1661	CD	PRO B	81		.854	-0.387	7.797
MOTA	1662	N	VAL B	82		.197	2.368	9.772
MOTA	1663	H	VAL B	82		.940	1.427	9.992
MOTA	1664	CA	VAL B	82		.380	3.306	10.885
MOTA	1665	С	VAL B	82		.160	2.668	12.010
MOTA	1666	0	VAL B	82		.045	1.465	12.293
MOTA	1667	CB	VAL B	82		.996	3.695	11.431
ATOM	1668	CG1	VAL B	82		.055	4.961	12.269
MOTA	1669	CG2	VAL B	82	10	. 958	3.857	10.318
ATOM	1670	N	ASN B	83	14	.963	3.422	12.775
ATOM	1671	Н	ASN B	83	15	.147	4.370	12.516
ATOM	1672	CA	ASN B	83	15	.550	2.846	13.967
ATOM	1673	C	ASN B	83		.481	2.874	15.022
ATOM	1674	Ö	ASN B	83		.814	3.903	15.294
ATOM	1675	СВ	ASN B	83		.743	3.639	14.472
ATOM	1676	CG	ASN B	83		.935	3.574	13.570
ATOM	1677	OD1		83		.409	2.511	13.167
ATOM	1678	ND2		83		.439	4.735	13.238
111011	10,0				_			





# Figure 11ee

MOTA	1679	2HD2	ASN B	83	19.237	4.786	12.638
MOTA	1680	1HD2	ASN B	83	18.030	5.580	13.582
MOTA	1681	N	ILE B	84	14.225	1.749	15.711
MOTA	1682	H	ILE B	84	14.791	0.938	15.564
MOTA	1683	CA	ILE B	84	13.154	1.658	16.667
MOTA	1684	С	ILE B	84	13.740	1.317	18.020
MOTA	1685	0	ILE B	84	14.428	0.300	18.223
ATOM	1686	CB	ILE B	84	12.214	0.517	16.260
MOTA	1687	CG1	ILE B	84	11.656	0.759	14.849
ATOM	1688	CG2	ILE B	84	11.128	0.247	17.315
ATOM	1689	CD1	ILE B	84	10.770	-0.359	14.291
ATOM	1690	N	ILE B	85	13.483	2.157	19.051
ATOM	1691	H	ILE B	85	13.028	3.030	18.877
ATOM	1692	CA	ILE B	85	13.846	1.834	20.408
ATOM	1693	C	ILE B	85	12.596	1.254	21.085
ATOM	1694	Ö	ILE B	85	11.536	1.903	21.267
ATOM	1695	CB	ILE B	85	14.308	3.115	21.137
ATOM	1696	CG1	ILE B	85	15.447	3.826	20.395
ATOM	1697	CG2	ILE B	85	14.673	2.840	22.589
ATOM	1698	CD1	ILE B	85	16.730	3.053	20.263
ATOM	1699	N	GLY B	86	12.617	-0.052	21.422
ATOM	1700	Н	GLY B	86	13.439	-0.595	21.251
ATOM	1701	CA	GLY B	86	11.481	-0.702	22.028
ATOM	1701	C	GLY B	86	11.557	-0.748	23.538
ATOM	1702	0	GLY B	86	12.412	-0.165	24.238
ATOM	1703	N	ARG B	87	10.614	-1.489	24.149
	1704	H	ARG B	87	10.014	-2.072	23.604
ATOM	1705		ARG B	87	10.442	-1.468	25.584
ATOM		CA C	ARG B	87	11.627	-2.021	26.326
ATOM	1707		ARG B	87	11.027	-1.666	27.495
ATOM	1708	O		87	9.200	-2.271	25.949
ATOM	1709	CB		87	7.951	-1.960	25.161
ATOM	1710	CG	ARG B		6.956	-3.074	25.219
ATOM	1711	CD	ARG B	87	5.906	-2.933	24.205
MOTA	1712	NE	ARG B	87		-2.933	23.772
MOTA	1713	HE	ARG B	87	5.790		
MOTA	1714	CZ	ARG B	87	5.119	-3.953	23.856
ATOM	1715	NH1	ARG B	87	5.252	-5.161	24.396 25.085
ATOM	1716	2HH1	ARG B	87	5.958	-5.326	24.113
ATOM	1717	1HH1	ARG B	87	4.646	-5.905	
ATOM	1718	NH2	ARG B	87	4.180	-3.751	22.939
ATOM	1719	1HH2	ARG B	87	3.580	-4.502	22.664
MOTA	1720	2HH2	ARG B	87	4.073	-2.848	22.524
MOTA	1721	N	ASN B	88	12.413	-2.937	25.731
MOTA	1722	H	ASN B	88	12.206	-3.237	24.800
ATOM	1723	CA	ASN B	88	13.582	-3.519	26.415
MOTA	1724	C	ASN B	88	14.532	-2.429	26.821
MOTA	1725	0	ASN B	88	15.214	-2.516	27.863
MOTA	1726	CB	ASN B	88	14.285	-4.605	25.559
MOTA	1727	CG	ASN B	88	15.063	-4.031	24.358
MOTA	1728	OD1	ASN B	88	14.515	-3.245	23.612
ATOM	1729	ND2	ASN B	88	16.333	-4.445	24.180
MOTA	1730	2HD2	ASN B	88	16.875	-4.099	23.414
MOTA	1731	1HD2	ASN B	88	16.744	-5.102	24.812
MOTA	1732	N	LEU B	89	14.695	-1.328	26.061
MOTA	1733	H	LEU B	89	14.192	-1.240	25.201
MOTA	1734	CA	LEU B	89	15.597	-0.234	26.452





# Figure 11ff

MOTA	1735	С	LEU B	89	14.797	0.937	27.053
ATOM	1736	0	LEU B	89	15.293	1.734	27.879
ATOM	1737	CB	LEU B	89	16.421	0.232	25.236
MOTA	1738	CG	LEU B	89	17.400	-0.754	24.567
ATOM	1739	CD1	LEU B	89	18.215	0.002	23.573
ATOM	1740	CD2	LEU B	89	18.352	-1.458	25.570
ATOM	1741	N	LEU B	90	13.511	1.114	26.705
ATOM	1742	H	LEU B	90	13.082	0.486	26.056
ATOM	1743	CA	LEU B	90	12.698	2.221	27.257
	1743	C	LEU B	90	12.537	2.060	28.751
ATOM		0			12.575	3.033	29.533
MOTA	1745		LEU B	90	11.311	2.258	26.628
MOTA	1746	CB	LEU B	90		2.730	25.168
ATOM	1747	CG	LEU B	90	11.232	2.744	24.642
ATOM	1748	CD1	LEU B	90	9.808		
ATOM	1749	CD2	LEU B	90	11.831	4.105	24.982
ATOM	1750	N	THR B	91	12.315	0.843	29.271
MOTA	1751	H	THR B	91	12.218	0.055	28.663
ATOM	1752	CA	THR B	91	12.210	0.634	30.699
ATOM	1753	C	THR B	91	13.537	1.028	31.375
MOTA	1754	0	THR B	91	13.575	1.525	32.518
MOTA	1755	CB	THR B	91	11.893	-0.843	31.028
ATOM	1756	OG1	THR B	91	12.919	-1.676	30.504
ATOM	1757	HG1	THR B	91	12.722	-2.634	30.713
ATOM	1758	CG2	THR B	91	10.599	-1.285	30.418
ATOM	1759	N	GLN B	92	14.705	0.852	30.732
ATOM	1760	H	GLN B	92	14.707	0.497	29.797
MOTA	1761	CA	GLN B	92	15.920	1.190	31.433
ATOM	1762	С	GLN B	92	16.088	2.660	31.633
ATOM	1763	0	GLN B	92	16.807	3.137	32.527
ATOM	1764	CB	GLN B	92	17.127	0.680	30.682
ATOM	1765	CG	GLN B	92	17.076	-0.805	30.517
ATOM	1766	CD	GLN B	92	18.336	-1.314	29.900
ATOM	1767	OE1	GLN B	92	19.394	-0.720	30.059
ATOM	1768	NE2	GLN B	92	18.221	-2.411	29.195
ATOM	1769	1HE2	GLN B	92	19.022	-2.813	28.751
ATOM	1770	2HE2	GLN B	92	17.331	-2.856	29.095
ATOM	1771	N	ILE B	93	15.538	3.512	30.746
ATOM	1772	H	ILE B	93	15.016	3.153	29.972
ATOM	1773	CA	ILE B	93	15.693	4.937	30.899
ATOM	1774	C	ILE B	93	14.522	5.549	31.698
ATOM	1775	Õ	ILE B	93	14.438	6.773	31.940
ATOM	1776	СВ	ILE B	93	15.981	5.657	29.548
ATOM	1777	CG1	ILE B	93	14.746	5.718	28.619
ATOM	1778	CG2	ILE B	93	17.223	5.060	28.874
ATOM	1779	CD1	ILE B	93	14.946	6.734	27.488
			GLY B	94	13.617	4.731	32.263
ATOM	1780	N			13.639	3.752	32.263
ATOM	1781	H		94			
ATOM	1782	CA	GLY B	94	12.594	5.224	33.170 32.432
ATOM	1783	C	GLY B	94	11.443	5.846	
ATOM	1784	O	GLY B	94	10.766	6.803	32.878
ATOM	1785	N	CYS B	95	11.134	5.354	31.225
ATOM	1786	H	CYS B	95	11.603	4.538	30.888
ATOM	1787	CA	CYS B	95	10.134	5.969	30.381
ATOM	1788	C	CYS B	95	8.750	5.512	30.764
ATOM	1789	O	CYS B	95 05	8.478	4.309	31.006
ATOM	1790	CB	CYS B	95	10.456	5.643	28.922





# Figure 11gg

ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1791 1792 1793 1794 1795 1796	SG N H CA C O CB	THR THR	В В В В	95 96 96 96 96	9.42 7.77 8.01 6.37 5.39	8 6.444 4 7.401 9 6.163 0 6.970 7 8.171	27.764 30.764 30.539 31.108 30.254 30.066
ATOM	1798	OG1	THR THR	В	96 96	6.11 6.34		32.604 32.938
ATOM	1799	HG1		В	96	6.11		33.861
MOTA	1800	CG2	THR	В	96	6.93		33.554
ATOM	1801	N	LEU	В	97	4.30		29.809
MOTA	1802	H	LEU	В	97	4.21	6 5.332	29.997
ATOM	1803	CA		В	97	3.12		29.238
ATOM	1804	C		В	97	2.33		30.358
ATOM	1805	0		В	97	2.35		31.499
ATOM	1806	CB		В	97	2.22		28.532
ATOM ATOM	1807 1808	CG CD1	LEU LEU		97	2.86		27.300
ATOM	1809	CD1		B B	97 97	2.10		26.957
ATOM	1810	N		В	98	2.84 1.63		26.085 30.024
ATOM	1811	H	ASN		98	1.66		29.063
ATOM	1812	CA	ASN		98	0.90		30.960
MOTA	1813	C	ASN		98	-0.25		30.231
MOTA	1814	0		В	98	-0.03		29.522
ATOM	1815	CB	ASN	В	98	1.84		31.587
ATOM	1816	CG		В	98	2.78	3 10.077	32.634
MOTA	1817	OD1		В	98	3.92	9.739	32.335
MOTA	1818	ND2		В	98	2.29	7 9.942	33.870
ATOM	1819	2HD2		В	98	2.87		34.599
ATOM	1820	1HD2		В	98	1.35		34.074
ATOM	1821	N		В	99	-1.47		30.426
ATOM ATOM	1822 1823	H CA		В	99	-1.56		31.037
ATOM	1824	CA		B B	99 99	-2.70		29.797
ATOM	1825	0		В	99	-3.81( -3.63(		30.815
ATOM	1826	CB		В	99	-3.14		32.011 28.657
ATOM	1827	CG		В	99	-3.71		28.941
ATOM	1828	CD1		В	99	-2.76		29.774
MOTA	1829	CD2		B	99	-5.13		29.528
MOTA	1830	OXT	LEU :	В	99	-4.842		30.376
TER								